National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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HECC Prioritizes Conservation of Environmental Resources in Operations

- The multiple modular supercomputing facilities that house the Electra and Aitken supercomputers produce an industry-leading annual Water Usage Effectiveness (WUE) of 0.21 liters (L) per kilowatt hour (kWh).
  - WUE is calculated as the (Annual Water Used) ÷ (IT Energy Used).
  - The U.S. Department of Energy reports the WUE of an average data center is 1.8 L per kWh.
  - The main facility in building N258 is about average, at 1.75 L per kWh. Continuous evaporation of tap water (drinking water) is the main heat transfer mechanism for cooling most data centers, like N258.
- Hybrid evaporative coolers for Electra and Aitken use water for cooling only when daytime temperatures rise.
  - Combined, the modules used 930,000 gallons of water supporting 1.9 megawatts (MW) of IT, while N258 used 15 million gallons of water supporting 3.7 MW of IT.
  - The Aitken supercomputer is supplied with 90-degree F cooling water, which permits extended dry operation and less water usage when evaporative cooling is required, yielding a WUE for the Aitken module of 0.10 L per kWh—a 94% reduction in WUE over N258 usage.
- As Aitken expands to meet the user community's needs, the facility will continue to prioritize water and energy savings.

IMPACT: HECC's use of hybrid evaporative coolers and warm water cooling allows NASA to wisely use water resources and greatly reduce water consumption for supercomputing operations.

The hybrid evaporative cooler next to the Aitken supercomputer module allows NASA to wisely use water resources. The Aitken and Electra coolers use water for cooling only when daytime temperatures rise and are dry through night and morning.
Derek Shaw, NASA/Ames

Control Room: A Year into Restricted Base Access

- Unlike most NASA staff, HECC's Control Room analysts (CRAs) have remained on site throughout the base access restrictions since March 9, 2020, assisting users and staff working from home.
- Many aspects of the work are unchanged from the period before the base access restrictions.
  - The team handled 25,235 user trouble tickets; and helped users with their configurations for new secure front ends and Aitken hardware.
  - The team implemented projects for continuous improvement, including a script documentation and update project. The updated scripts improved error handling of job submissions by identifying misconfigured resource requests.
- New CRA work centers mainly around HECC support teams who need onsite support and safety protocols.
  - The CRAs assumed a greater role in the monthly patch cycle for Enterprise System Support, and more system administrator tasks such as advanced reservations and node diagnostics for Systems Support.
  - The CRAs were instrumental in monitoring, maintaining, procuring, and setting up Personal Protective Equipment (PPE) throughout building N258 for the safety of those working and visiting the facility. This allowed all those within the building to continue to provide uninterrupted essential functions of the HECC systems during the COVID-19 pandemic, such as monitoring of all systems, supporting supercomputer end-users, conducting safety walkthroughs, and facilitating critical shipments to maintain the various systems within the facility.
- The CRAs were nominated for an Ames Honor Award and received the Ames Safety Award for their service through the restricted base access.

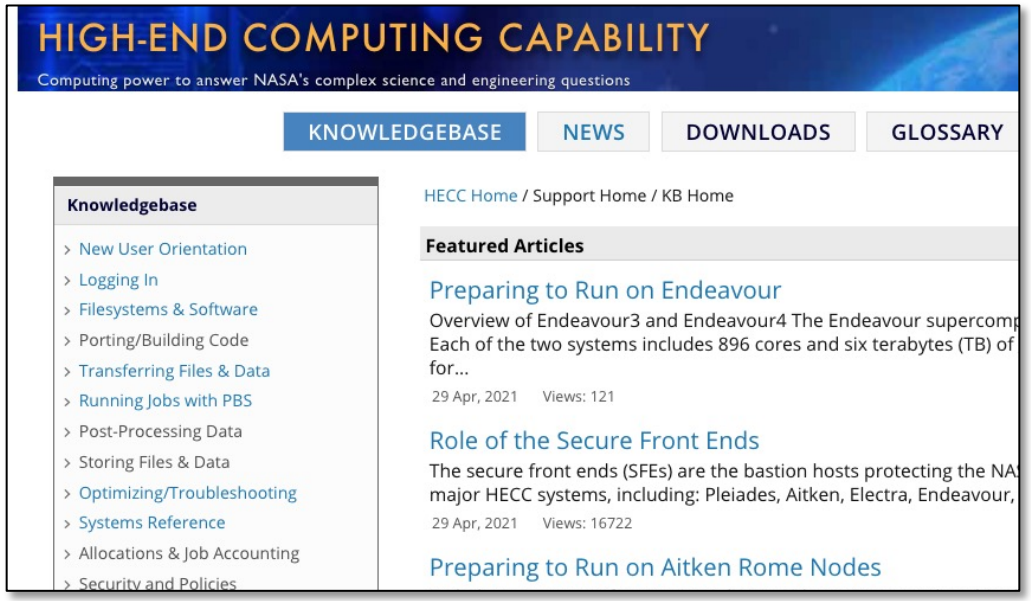
IMPACT: HECC's Control Room Analysts enable researchers to better utilize NASA's supercomputing resources for their modeling and simulation projects, supporting the agency's mission goals.

HECC's Control Room team provides a variety of services aimed at maximizing users' allocations on the supercomputing resources and providing support to users and support staff across multiple centers. *NASA Ames*

Knowledge Base Revised to Support New HECC Hardware

- The HECC Knowledge Base (KB) was significantly revised over the past several months in order to incorporate three major updates to the HECC supercomputing environment.
- The HECC Publications & Media team worked closely with the Application Performance and Productivity (APP) team to update more than 75 articles and add several new articles since January 2021, to support the addition of Aitken's Rome nodes and the decommissioning, replacement of Endeavour and the secure front-end systems (SFEs).
  - The updates provide HECC users with the information they need to access the new systems, compile code, run jobs, and troubleshoot issues; as well as how to use new features, such as the ability to log into the secure enclave using a NASA PIV badge with RSA SecurID.
  - Extensive research by the APP team was required to determine specific new documentation needed to support the new hardware, especially the AMD Rome nodes—a completely new architecture introduced into the HECC environment.
  - In addition to the recent changes, the teams have added approximately 70 new articles since June 2019 to support the initial deployment of Aitken; new V100 GPU nodes; new offerings such as AWS cloud, Jupyter, and Singularity; and new optimization tools and methods.

IMPACT: The HECC Knowledge Base (KB) provides the technical documentation NASA researchers and engineers need to effectively use HECC resources, including the Pleiades, Aitken, Electra, and Endeavour supercomputers. Averaging more than 5,000 article views each week, the KB is an invaluable resource to users.

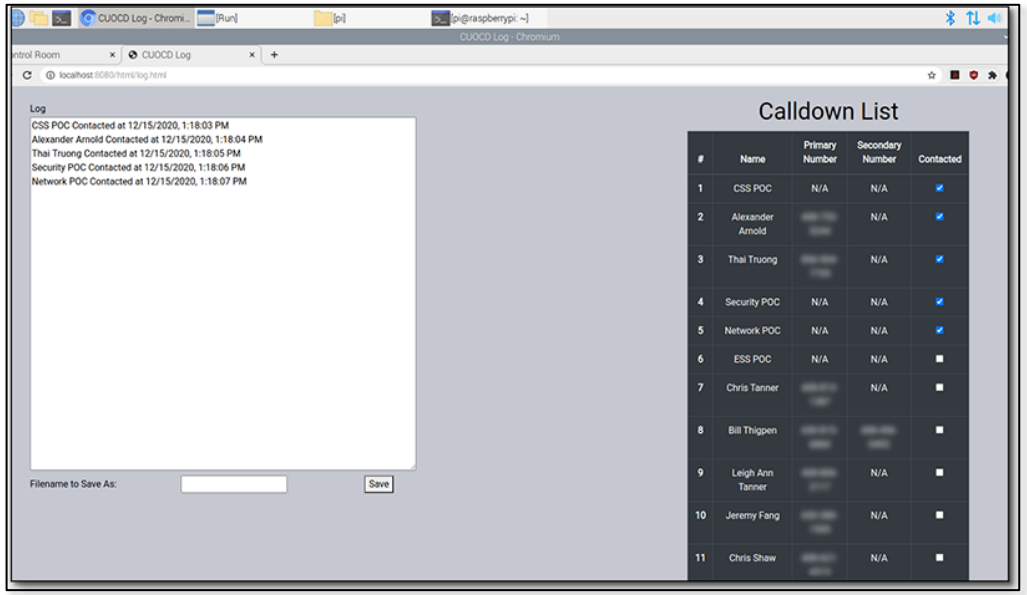


Home page of the HECC Knowledge Base (KB), which provides comprehensive user documentation for all of the supercomputing resources managed by the HECC Project. Currently, there are more than 360 technical articles published in the KB.

HECC Team Improves Critical Unplanned Outage Communication Process

- The Critical Unplanned Outage Communication Design (CUOCD) project team developed a Raspberry Pi-based software tool and process for communications during critical outages. The CUOCD user interface (UI) simplifies a process with many input variables and potential outcomes into an easy-to-follow straightforward list of instructions for Control Room staff. This reduces potential confusion and allows for faster emergency response.
- The CUOCD UI general process is as follows:
  - Control Room staff make selections in the UI (System, Issue, Trigger).
  - The UI generates a call-down list of instructions for both management and technical POCs.
  - Control Room staff follow the listed instructions and log events into the UI (who is called, when emails are sent, final all-clear notification).
  - This log is then transferred over to the Remedy logbook with the provided timestamps.
- This first iteration of the project will be the foundation for building future features to further increase the utility of the tool. Potential new features include automated email of logs, tracking of events outside of the Control Room, and addition of an uninterruptible power supply to resist power outage events.

IMPACT: HECC's new user interface simplifies actions and decisions needed for keeping stakeholders informed during critical outages, replacing historically disparate and separately managed procedures. The new process leads to fewer errors and greater accuracy in event tracking.

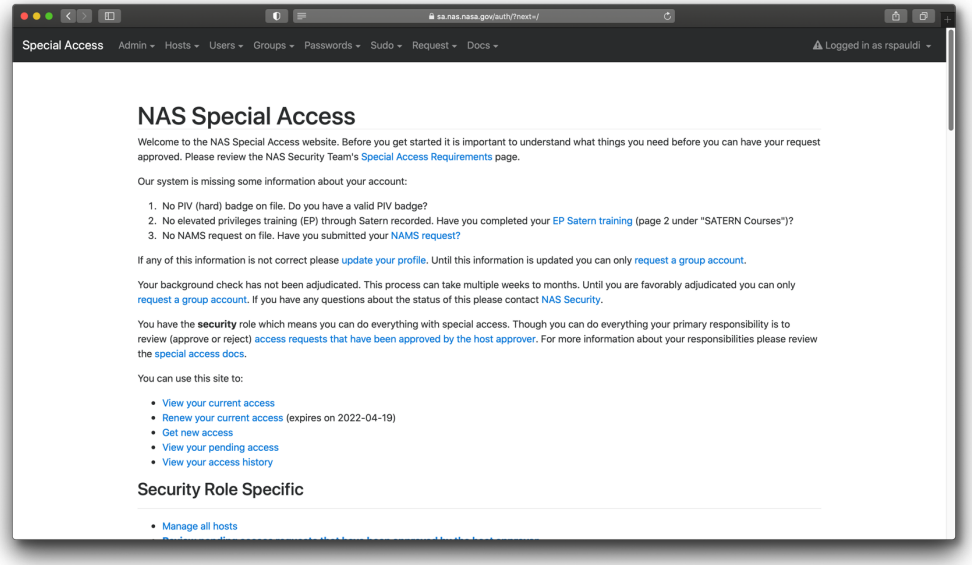


Example call-down list generated by the Critical Unplanned Outage Communication user interface.

HECC Improves Special Access Website Processes

- The NAS Special Access website allows staff to make additional requests for administrative functions. Recently, some updates were made to the system, along with process improvements that free staffing resources.
  - The Tools team assumed management of the Special Access website, previously maintained by the HECC Security team.
  - Control Room staff are now responsible for quarterly Special Access tasks.
- The Tools team designed some key changes to the new website, including:
  - An improved user interface (UI) allows users to view and edit previous requests.
  - Through the UI, users can now see the status of their requests prior to approval by management and the NAS Security Team.
- Moving forward, the Tools team will handle ongoing improvements and updates, with a focus on improving the user experience.

IMPACT: Shifting the responsibilities of maintaining the Special Access website to other teams allows the HECC Security team to focus its resources on more critical work and allots other resources to make improvements to the user experience.

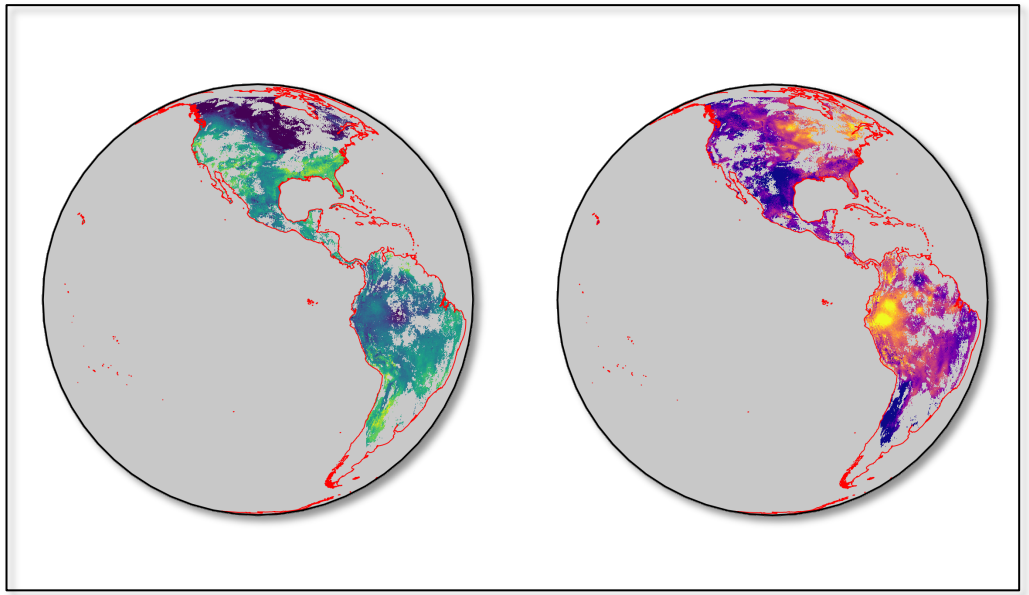


Sample screenshot of the NAS Special Access website.

Application Experts Improve Performance of Satellite Data-Processing Code

- HECC's Applications Performance and Productivity (APP) team recently achieved a 15% performance improvement for a code that will be used to produce Level-2 data for a satellite mission.
  - The Geostationary Carbon Observatory (GeoCarb) mission will collect 4 million daily atmospheric soundings of greenhouse gas concentrations and solar-induced fluorescence at a spatial resolution of about 3 by 6 kilometers.
  - The GeoCarb Level 2 Full Physics algorithm will be used to process approximately 1 million cloud-free soundings to retrieve column concentrations of carbon dioxide, methane, and carbon monoxide.
- The APP team used a variety of tools to locate performance bottlenecks. The optimization technique most responsible for the improvement was to rearrange numerous regions of memory to improve cache line usage.
- The 15% improvement equates to 150,000 SBUs/year at the rate the project is expected to consume resources when in production. Heather Cronk, project scientist at Colorado State University said, "A 15% speed up when we are talking a million runs every day is incredible. It will help us meet latency requirements, in addition to making us much better stewards of HECC processing hardware."

IMPACT: Performance enhancements to heavily used codes not only improve the time to solution for the projects' workflow, but also result in system resources being available for other work.



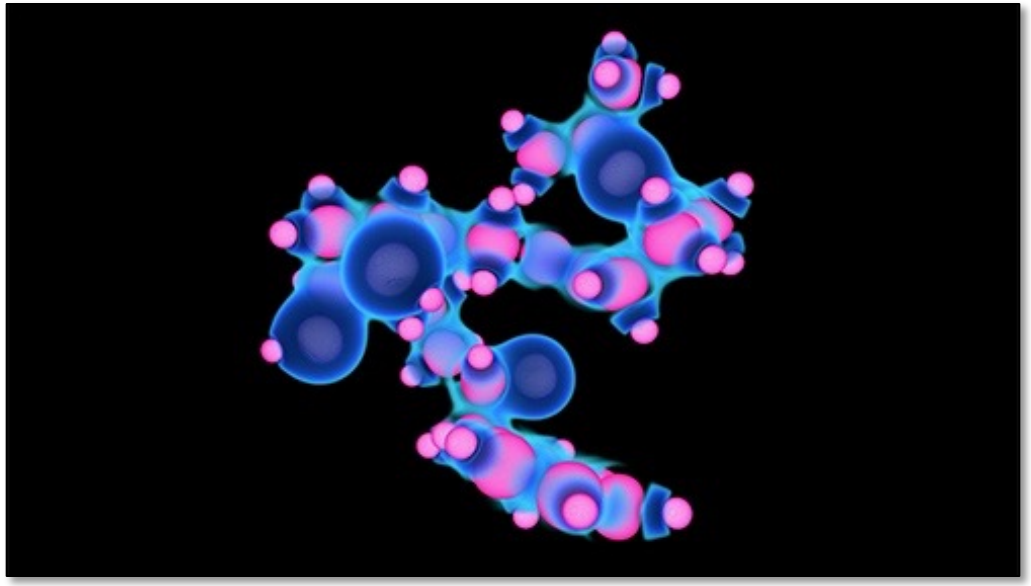
Column concentrations of carbon dioxide and methane retrieved by the GeoCarb Level 2 Full Physics algorithm for the Day in the Life Test #2.
Peter Somkuti, Cooperative Institute for Research in the Atmosphere, Colorado State University

Using 3D-Aware Machine Learning for Drug Repurposing in COVID-19 Research*

- Researchers from Harvard University and Massachusetts Institute of Technology used machine learning models on NASA's high-end computing resources to find leads for novel therapeutics against pathogens like SARS-CoV-2, the virus responsible for COVID-19, and to predict drug activity. Their work investigates whether machine learning predictions can be improved using interconverting 3D structure (conformers) ensemble representation of molecules.
- With a dataset of 304,466 drug-like molecules and 133,318 combinatorially generated molecules, the team used the newly developed Conformer-Rotamer Ensemble Sampling Tool (CREST) software to generate conformers for each species, leading to over 33 million conformers. They then trained a model on 278,793 molecules for inhibition to a SARS-CoV protease, used the trained model to generate fingerprints for 837 molecules that have tested for inhibition, and a new network was trained to predict inhibition from these fixed fingerprints.
- Results from this work show that 3D information improves the receiver operating characteristic and the precision-recall curve when compared to 2D models.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: This work was part of the COVID-19 HPC Consortium, which provided high-performance computing access to researchers around the world studying the global transmission and impact of the COVID-19 virus.



CREST simulation of the latanoprost molecule. A quantum chemistry calculation is performed at each step, yielding the energy, charge density, and atomic forces. The calculation is used as input to a meta-dynamics step, which accelerates the atoms in the direction of the forces while biasing them towards new conformations. Warm colors signify charge concentration and cool colors signify charge depletion. *Chris Henze, NASA/Ames*

Papers

- "**Seasonal Blooms of the Dinoflagellate Algae Noctiluca scintillans: Regional and Global Scale Aspects**," S. Piontkovski, et al., Regional Studies in Marine Science, vol. 44, published online April 5, 2021. * *https://www.sciencedirect.com/science/article/abs/pii/S2352485521001638*
- "**Resolving Pitching Airfoil Transonic Aerodynamics by CFD Data Modeling**," U. Kaul, Journal of Fluids Engineering, published online April 7, 2021. * *https://asmedigitalcollection.asme.org/fluidsengineering/article/doi/10.1115/1.4050800/1106713/Resolving-Pitching-Airfoil-Transonic-Aerodynamics*
- "**Multimessenger Binary Mergers Containing Neutron Stars: Gravitational Waves, Jets, and *γ*-Ray Bursts**," M. Ruiz, S. Shapiro, A. Tsokaros," Frontiers in Astronomy and Space Sciences, April 8, 2021. * *https://www.frontiersin.org/articles/10.3389/fspas.2021.656907/full*
- "**Erosion of Refractory Carbides in High-Temperatures Hydrogen from Ab Initio Computations**," W. Tucker, et al., Journal of the American Ceramic Society, published online April 12, 2021. * *https://ceramics.onlinelibrary.wiley.com/doi/abs/10.1111/jace.17844*
- "**Hot Planets Around Cool Stars – Two Short-Period Mini-Neptunes Transiting the Late K-Dwarf TOI-1260**," I. Y. Georgieva, et al., arXiv:05653 [astro-ph.EP], April 12, 2021. * *https://arxiv.org/abs/2104.05653*

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Multi-Fluid MHD-Simulations of Europa's Plasma Interaction Under Different Magnetospheric Conditions**," C. Harris, et al., Journal of Geophysical Research: Space Physics, vol. 126, issue 5, April 14, 2021. * *https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2020JA028888*
- "**Nonlinear Coupling of Whistler Waves to Oblique Electrostatic Turbulence Enabled by Cold Plasma**," V. Roytershteyn, G. L. Deizanno, Physics of Plasmas, vol. 28, issue 4, published online April 19, 2021. * *https://aip.scitation.org/doi/full/10.1063/5.0041838*
- "**Microjet Configuration Sensitivities for Active Flow Control on Multi-Element High-Lift Systems**," S. S. Hosseini, A. Cooperman, C. van Dam, S. Pandya, Journal of Aircraft, published online April 21, 2021. * *https://arc.aiaa.org/doi/abs/10.2514/1.C035986*
- "**Five Years of Variability in the Global Carbon Cycle: Comparing an Estimate from the Orbiting Carbon Observatory-2 and Processes-Based Models**," Z. Chen, et al., Environmental Research: Letters, published online April 22, 2021. * *https://iopscience.iop.org/article/10.1088/1748-9326/abfac1/meta*
- "**TOI-1431b/MASCARA-5b: A Highly Irradiated Ultra-Hot Jupiter Orbiting One of the Hottest & Brightest Known Exoplanet Host Stars**," B. C. Addison, et al., arXiv:2104.12078 [astro-ph.EP], April 25, 2021. * *https://arxiv.org/abs/2104.12078*

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Papers (cont.)

- "**A Transiting Warm Giant Planet around the Young Active Star TOI-201**," M. Hobson, et al., The Astronomical Journal, vol. 161, no. 5, April 26, 2021. *
  https://iopscience.iop.org/article/10.3847/1538-3881/abeaa1
- "**Investigating Lack of Accretion Disk Eccentricity Growth in a Global 3D MHD Simulation of a Superhump System**," B. Oyang, Y.-F. Jiang, O. Blaes, Monthly Notices of the Royal Astronomical Society, April 30, 2021. *
  https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stab1212/6261206
- "**Dutch-Roll Stability Analysis of an Air Mobility Vehicle Using Navier-Stokes Equations**," G. Guruswamy, AIAA Journal, published online April 30, 2021. *
  https://arc.aiaa.org/doi/full/10.2514/1.J060055
- "**Cross-Comparison of Global Simulation Models Applied to Mercury's Dayside Magnetosphere**," S. Aizawa, et al., Planetary and Space Science, vol. 198, April 2021. *
  https://www.sciencedirect.com/science/article/pii/S0032063321000155

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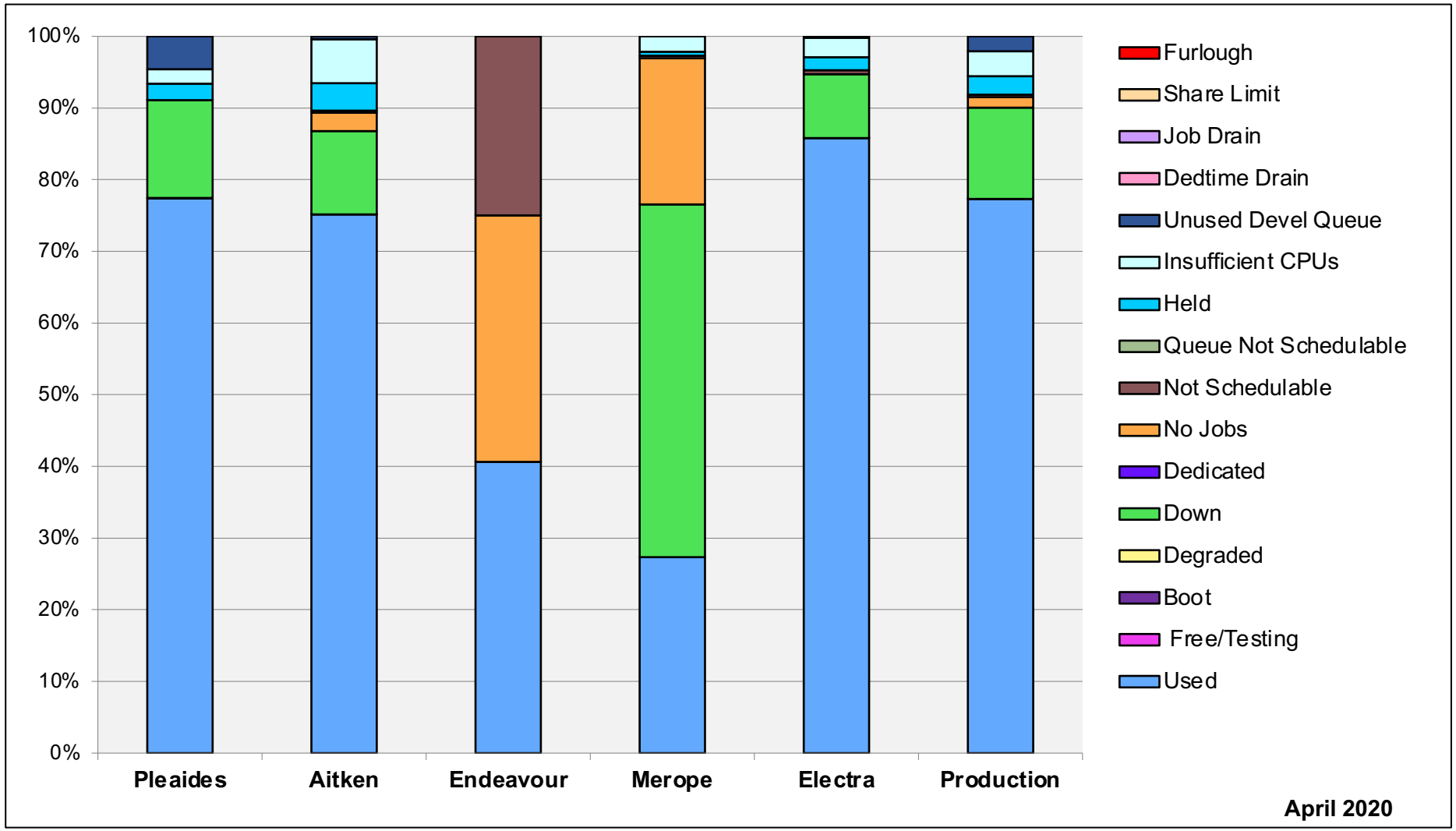
News and Events

- **Saving Earth from Asteroids**, *NASA Feature*, April 23, 2021–Using simulations run on systems at the NASA Advanced Supercomputing Facility, researchers are working on how to measure the impact of an asteroid that may be getting too close to Earth for comfort.
  https://www.nasa.gov/feature/saving-earth-from-asteroids
- **Binary Black Hole Simulations Provide Blueprint for Future Observations**, *Cutting Edge*, NASA Goddard Space Flight Center, Spring 2021—A NASA Goddard astronomer hopes his black hole simulations will help future missions home in on black holes, the most elusive inhabitants of the universe. Simulations were run on the Pleiades supercomputer.
  https://issuu.com/nasagsfc/docs/spring_2021_final_web_version/s/12129994

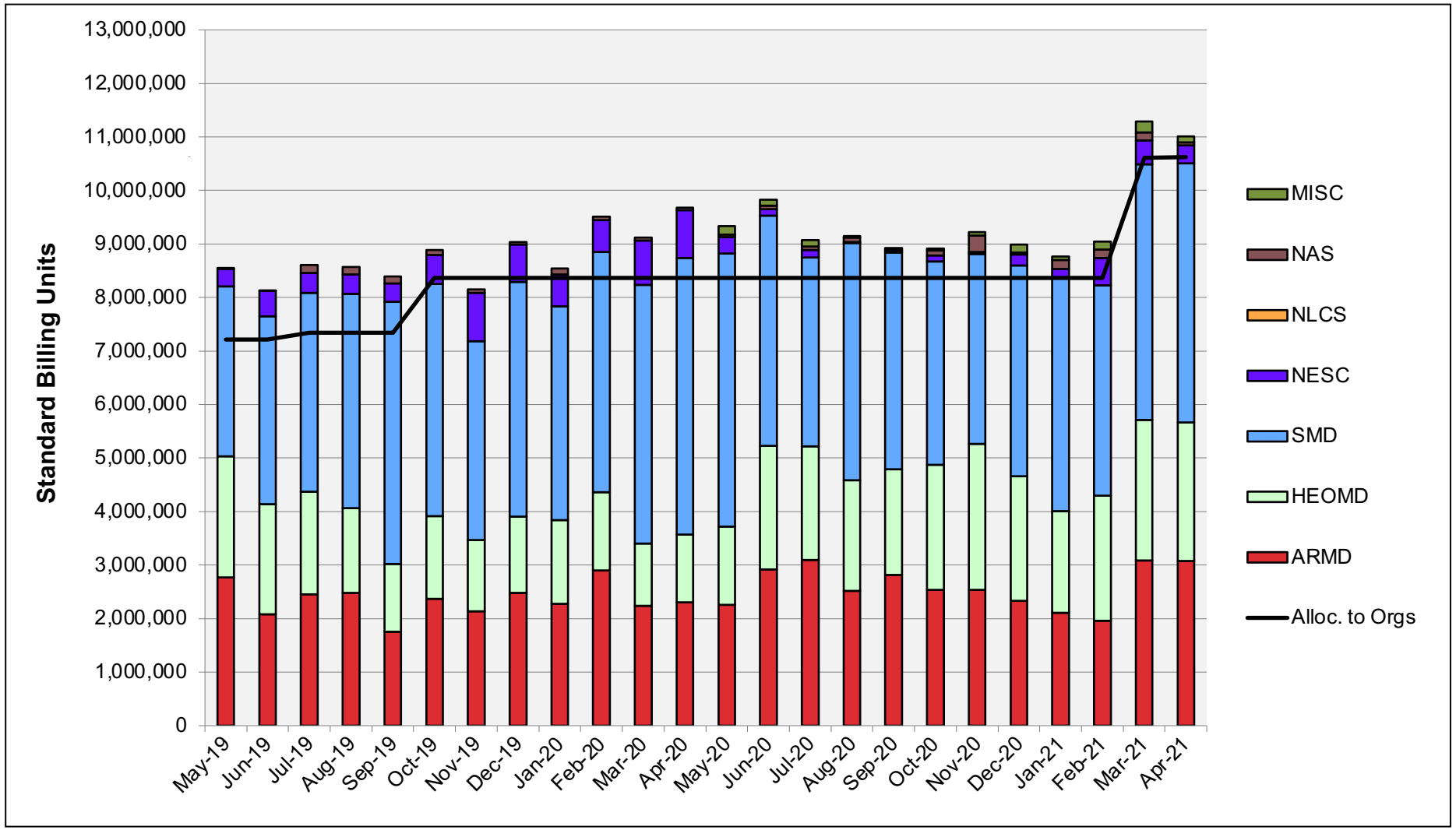
News and Events: Social Media

- **Coverage of NAS Stories**
  - #EarthDay NASA Campaign:
    - NASA Supercomputing: Twitter 4 retweets, 8 likes; Facebook 291 users reached, 41 engagements, 8 likes, 5 shares.
    - NAS: Twitter 1 retweet, 4 likes.
  - #BlackHoleWeek NASA Campaign:
    - NASA Supercomputing: Twitter 119 retweets, 9 quote tweets, 562 likes; Facebook 136 users reached, 11 engagements, 3 likes, 2 shares.
  - Mars Ingenuity Flight-related:
    - NASA Supercomputing: Twitter 1 retweet, 6 likes; Facebook 350 users reached, 21 engagements, 9 likes, 4 shares.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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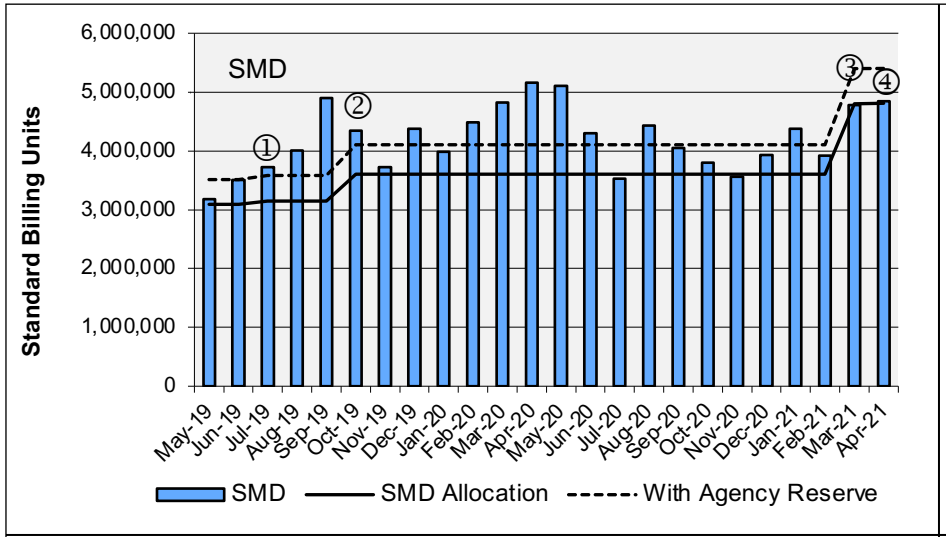
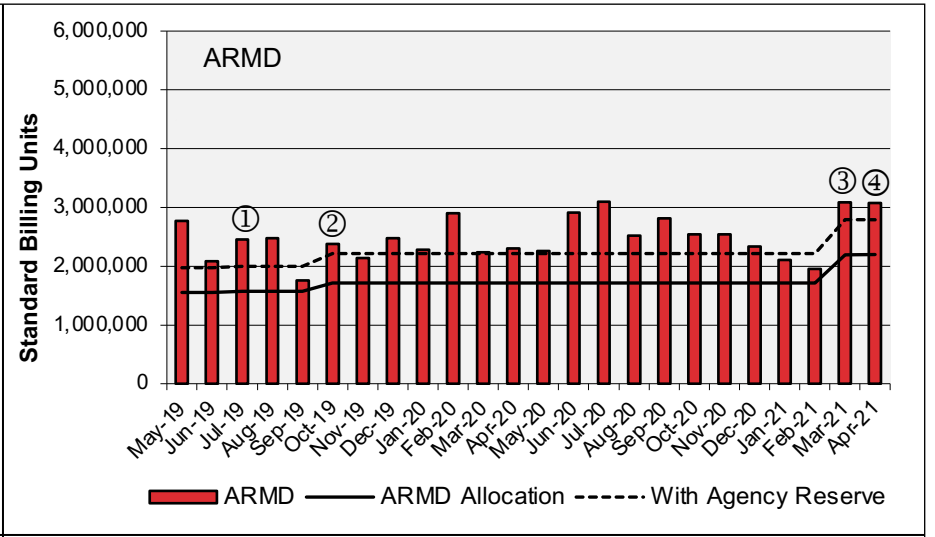
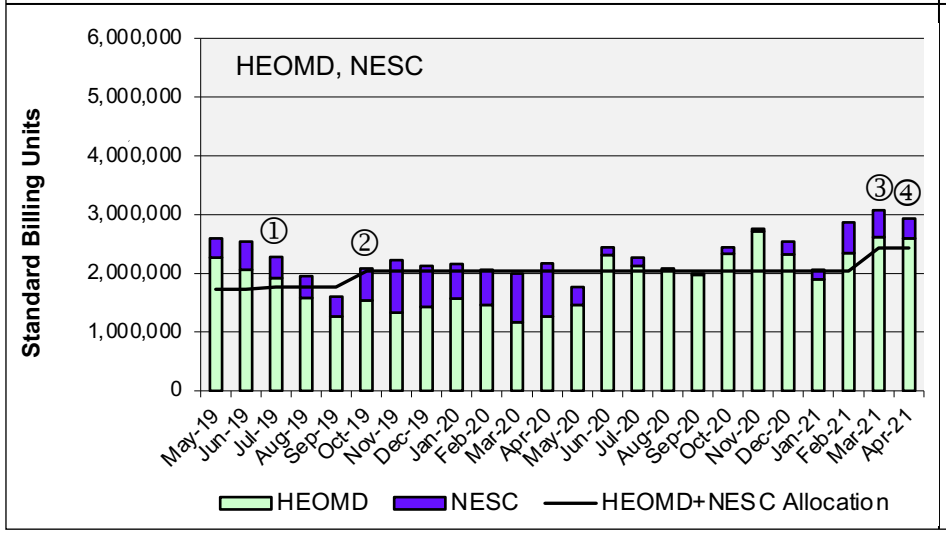






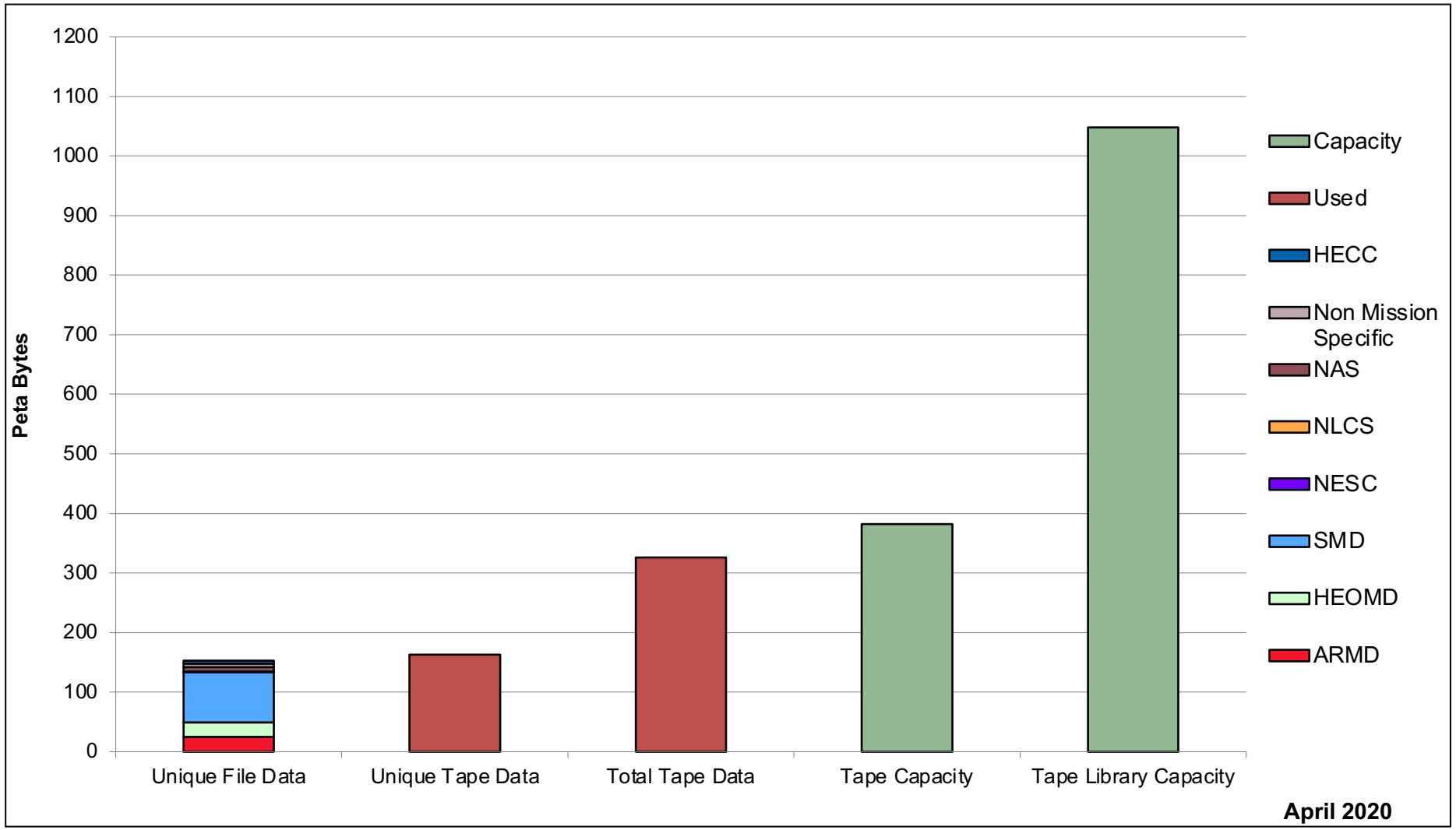
① Skylake Tesla GPU V100 Nodes installed

② 4 Cascade Lake E cells introduced into Aitken

③ 8 Rome Apollo racks introduced into Aitken

④ Endeavour replaced with new hardware

Tape Archive Status



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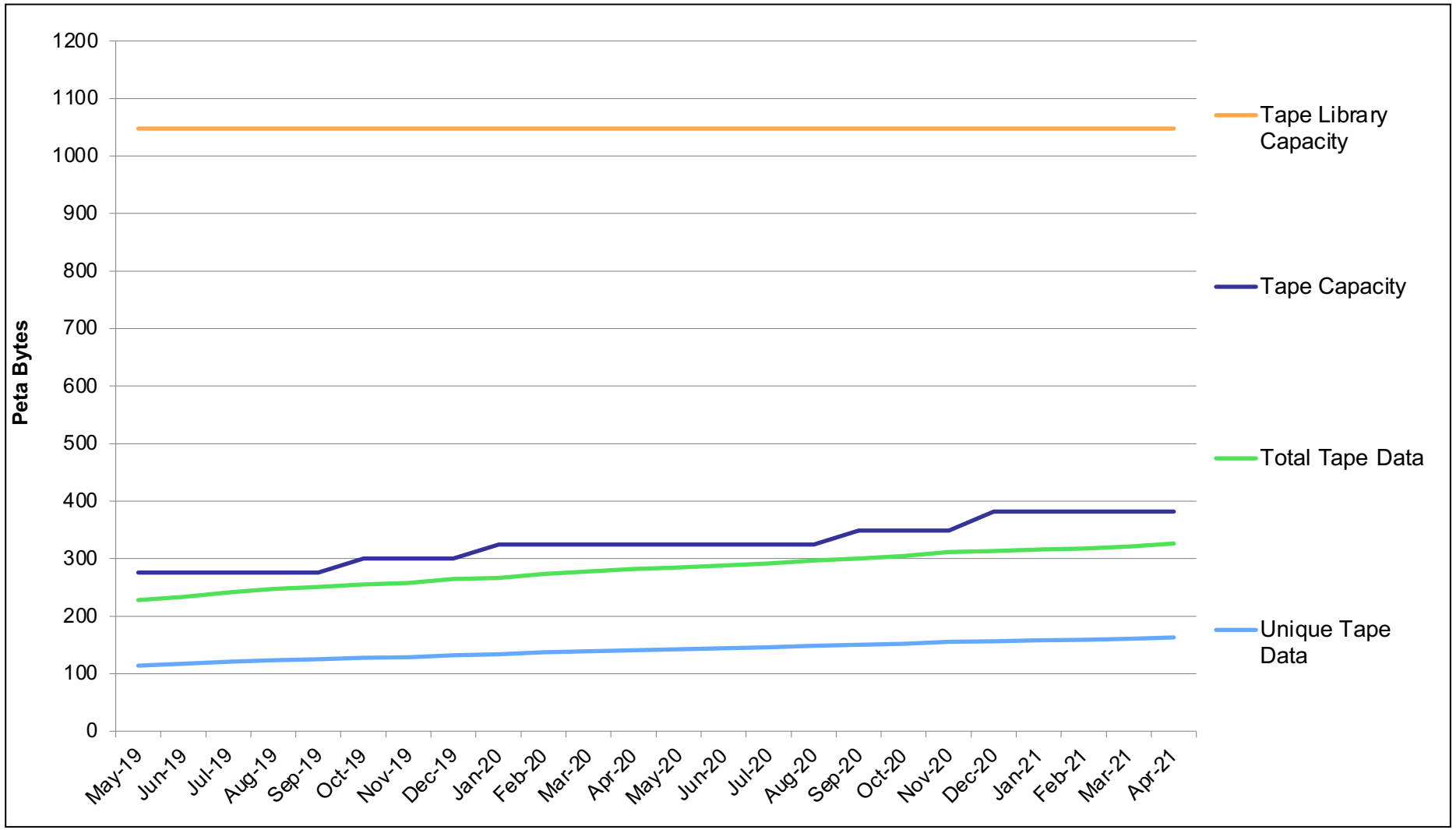
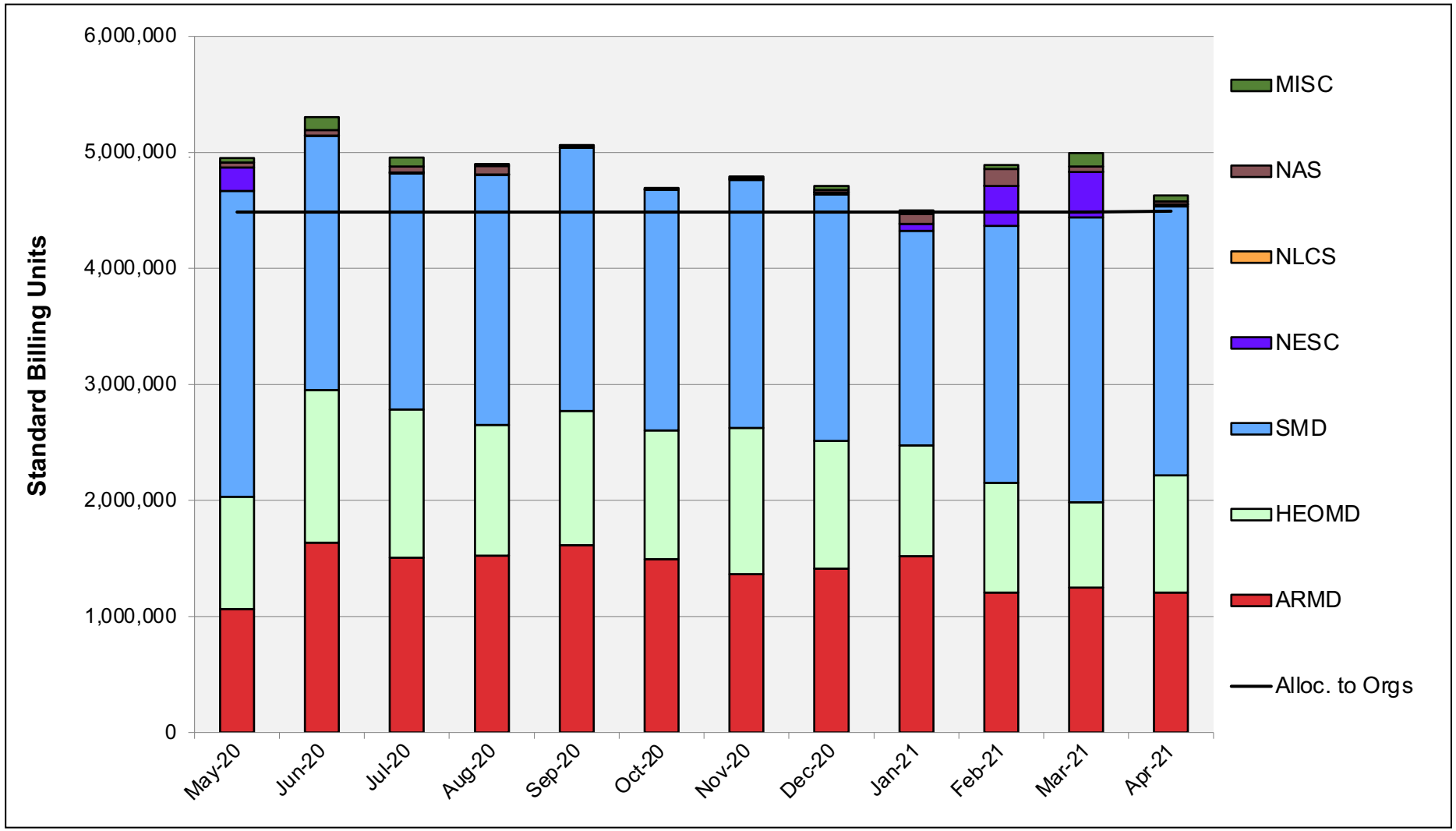
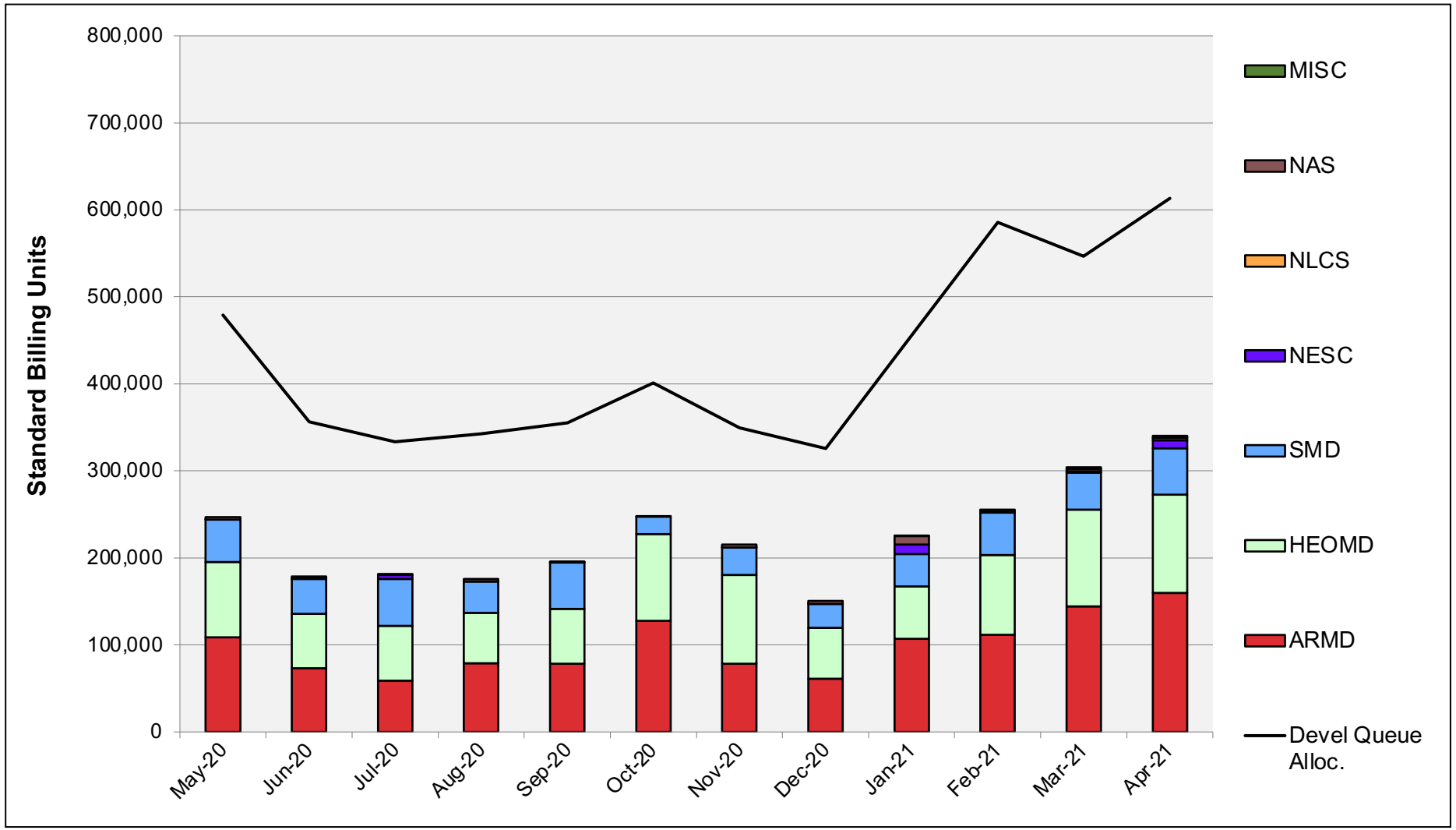


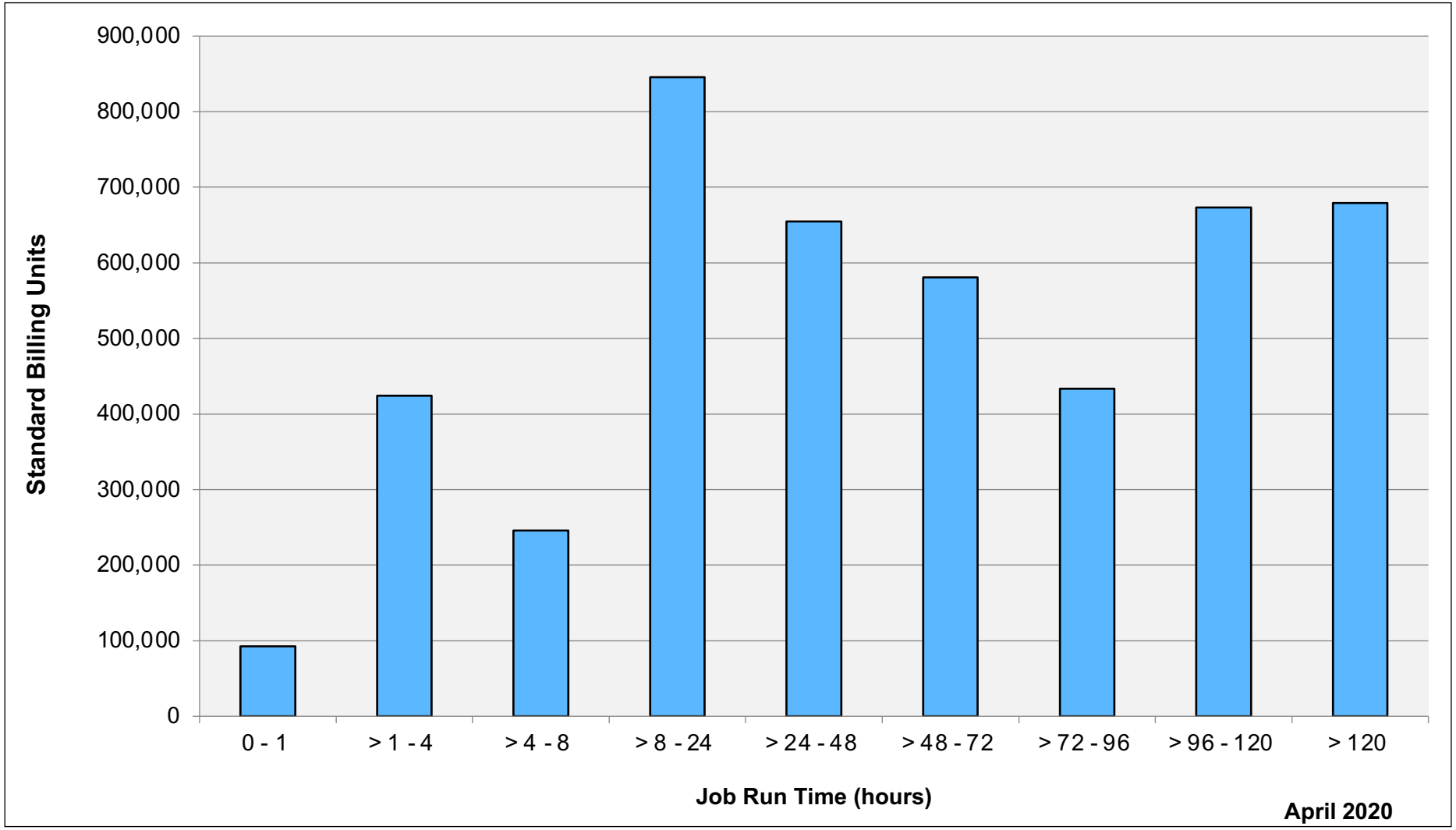
Pleiades: SBUs Reported, Normalized to 30-Day Month



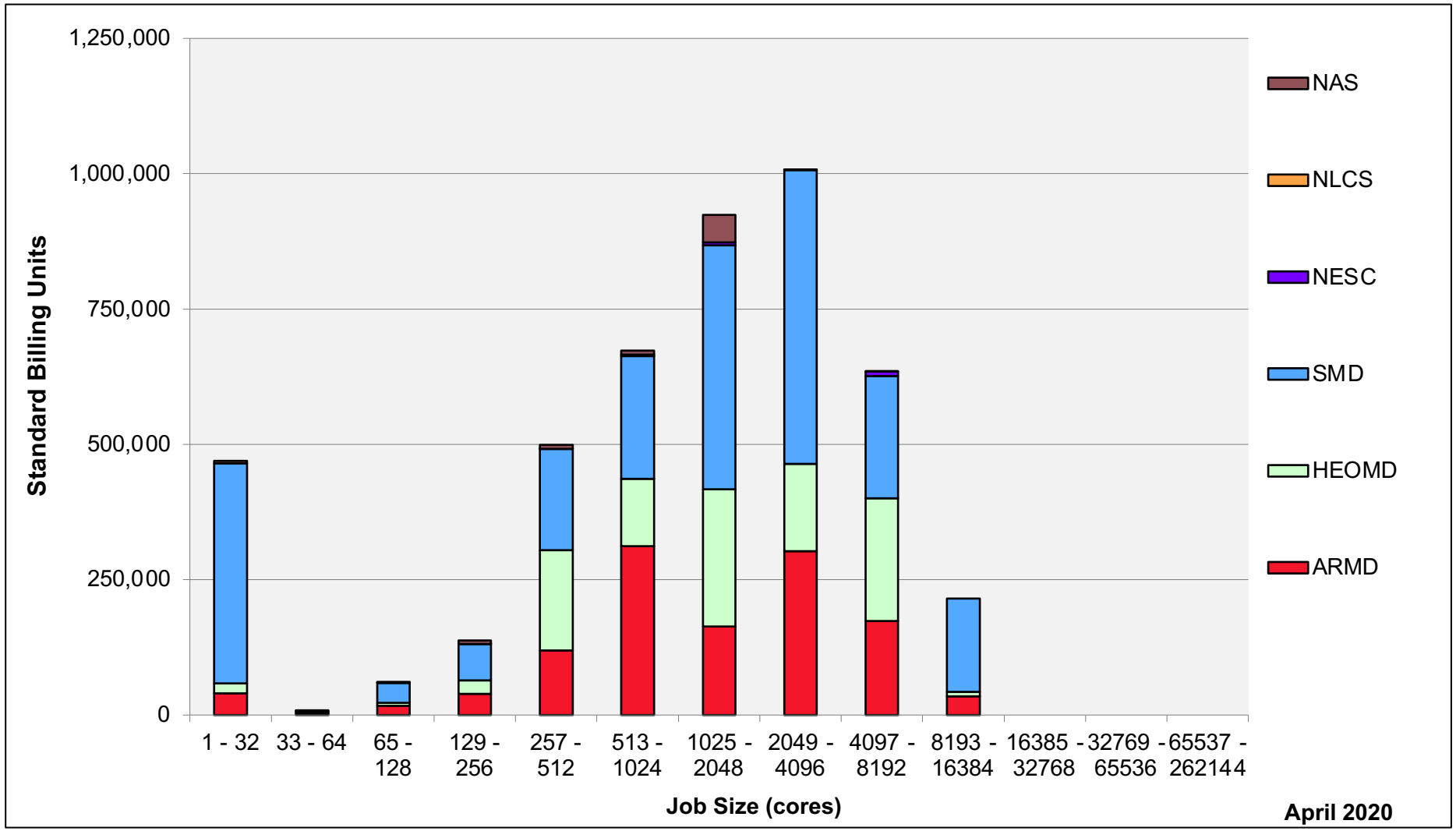
Pleiades: Devel Queue Utilization



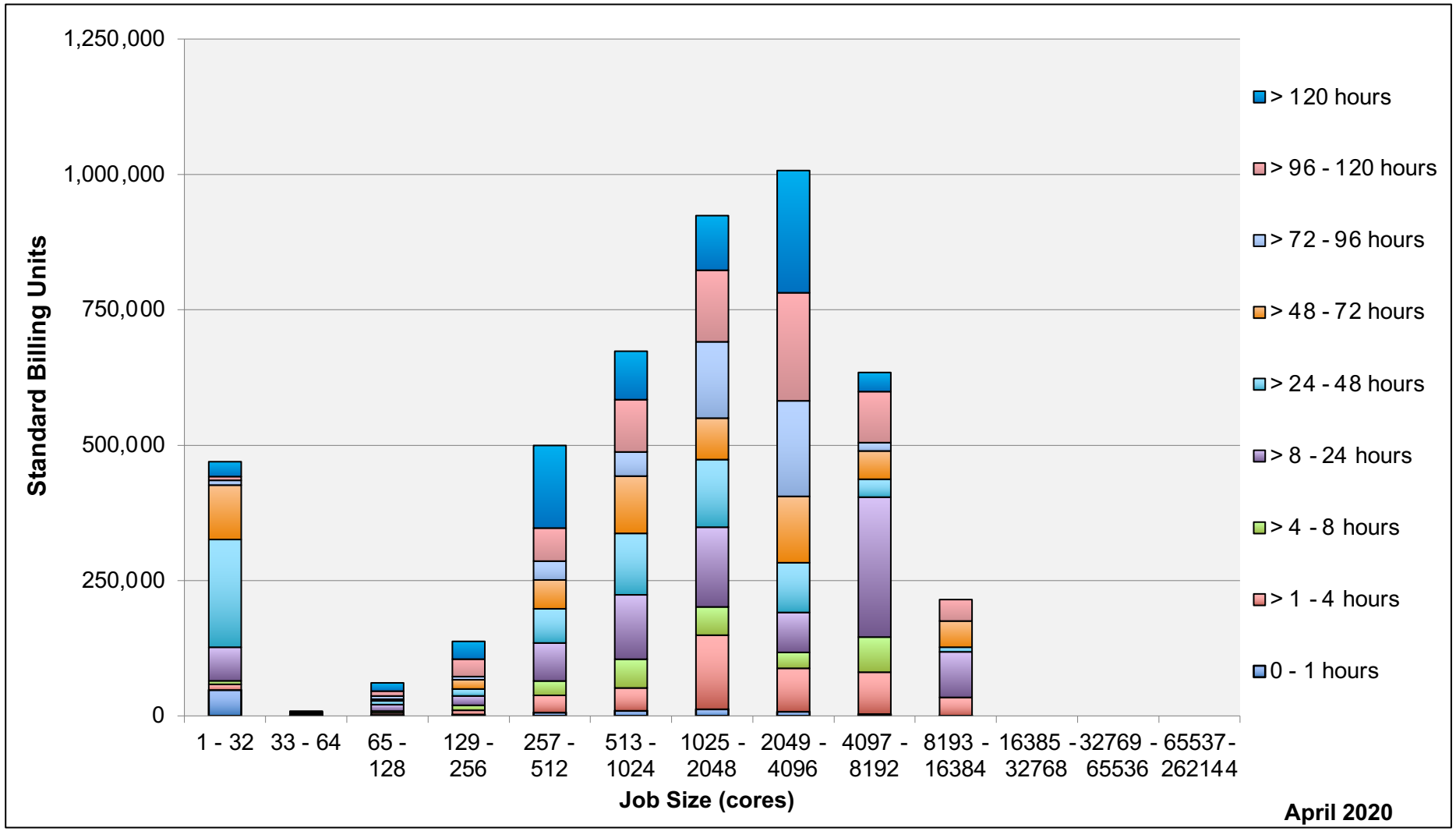
Pleiades: Monthly Utilization by Job Length



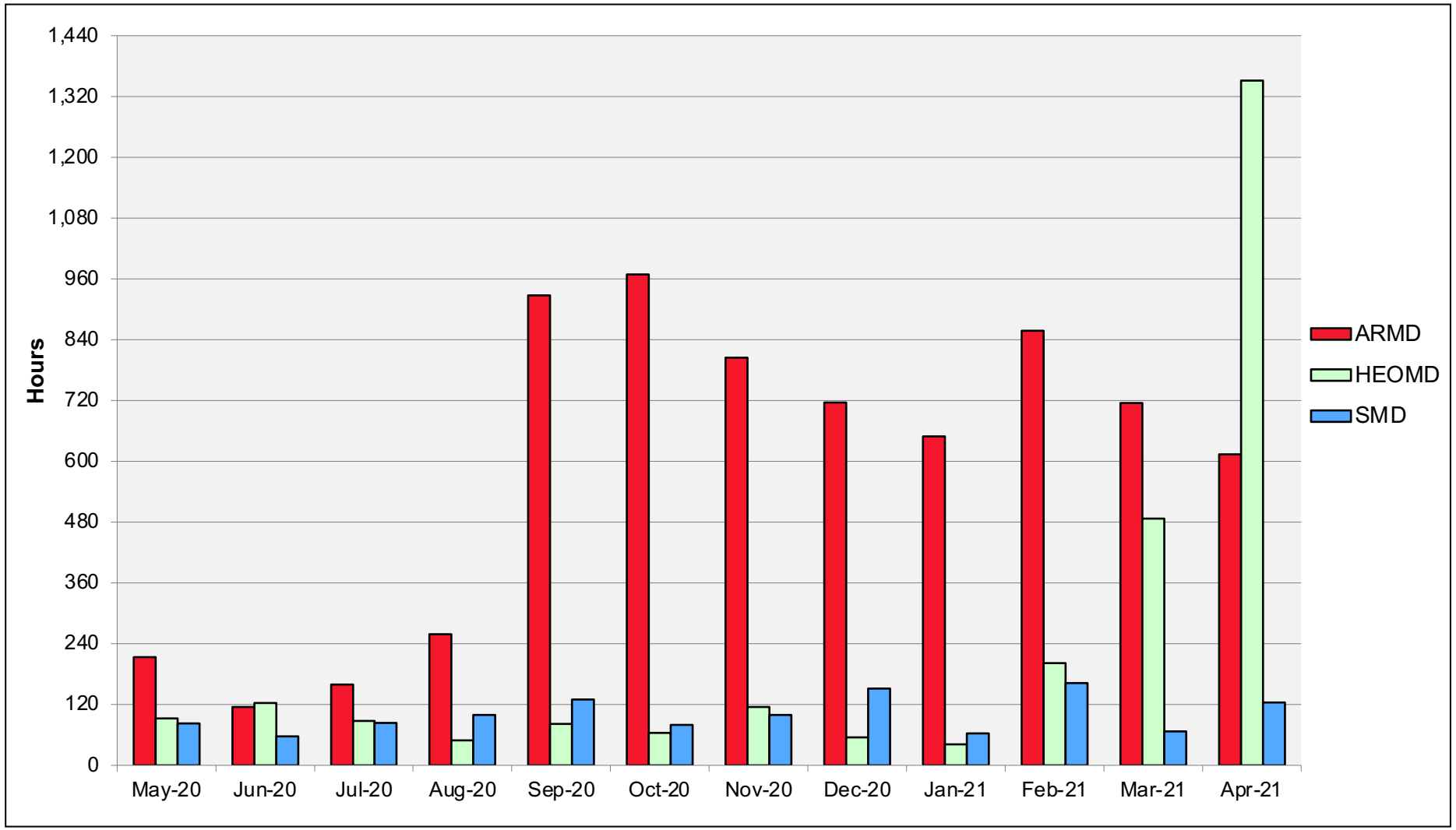
Pleiades: Monthly Utilization by Job Size



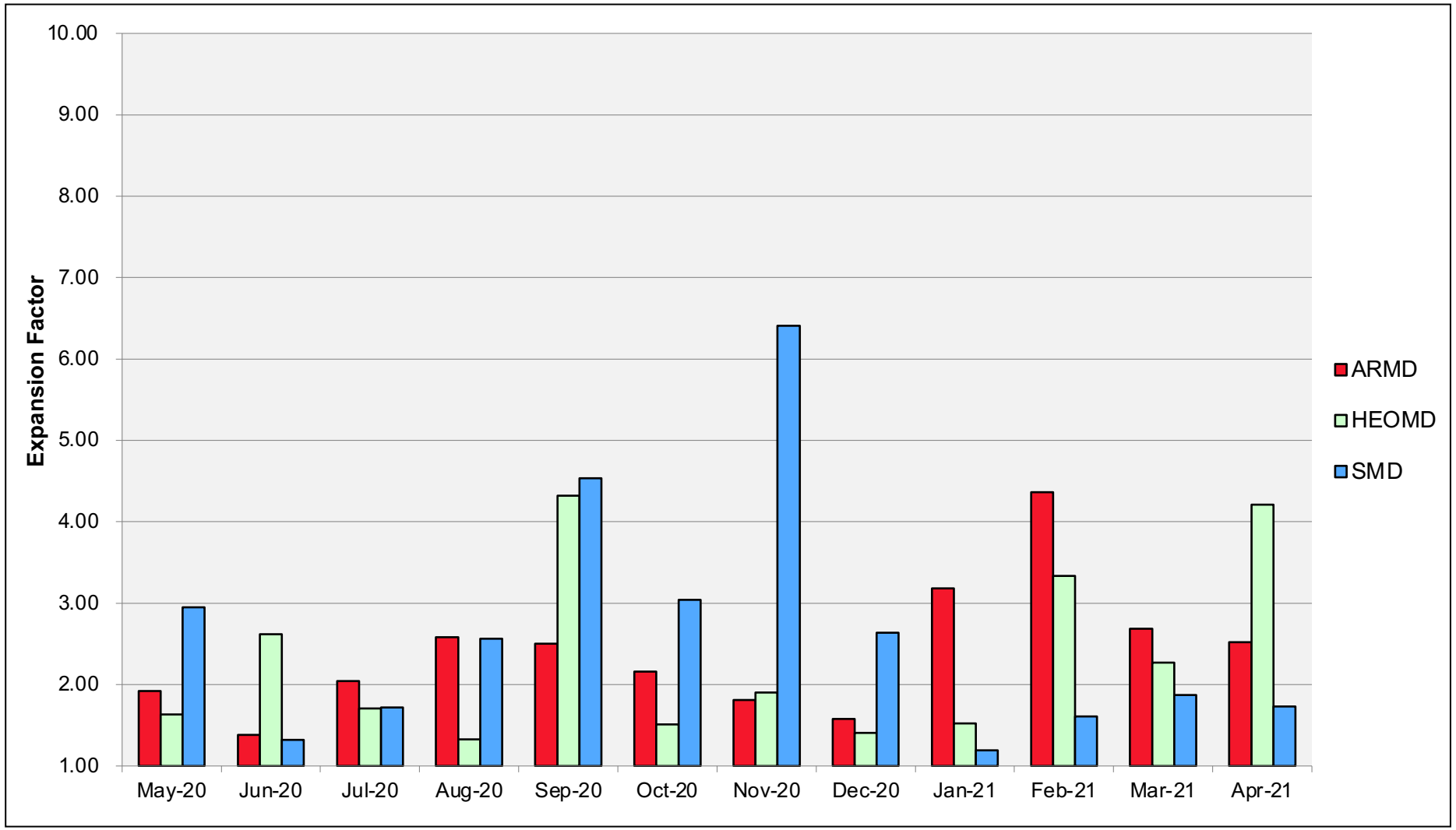
Pleiades: Monthly Utilization by Size and Length



Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



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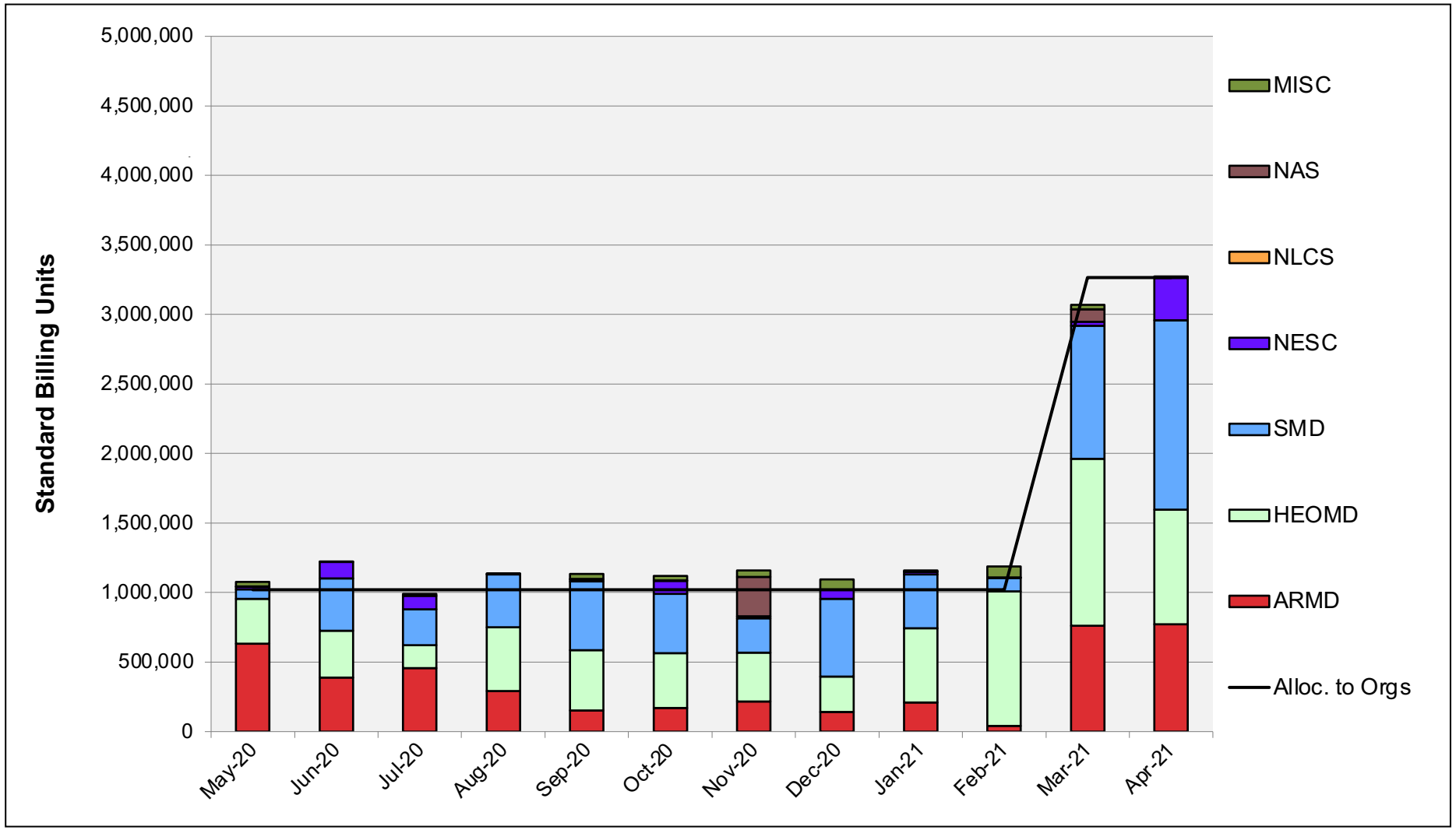

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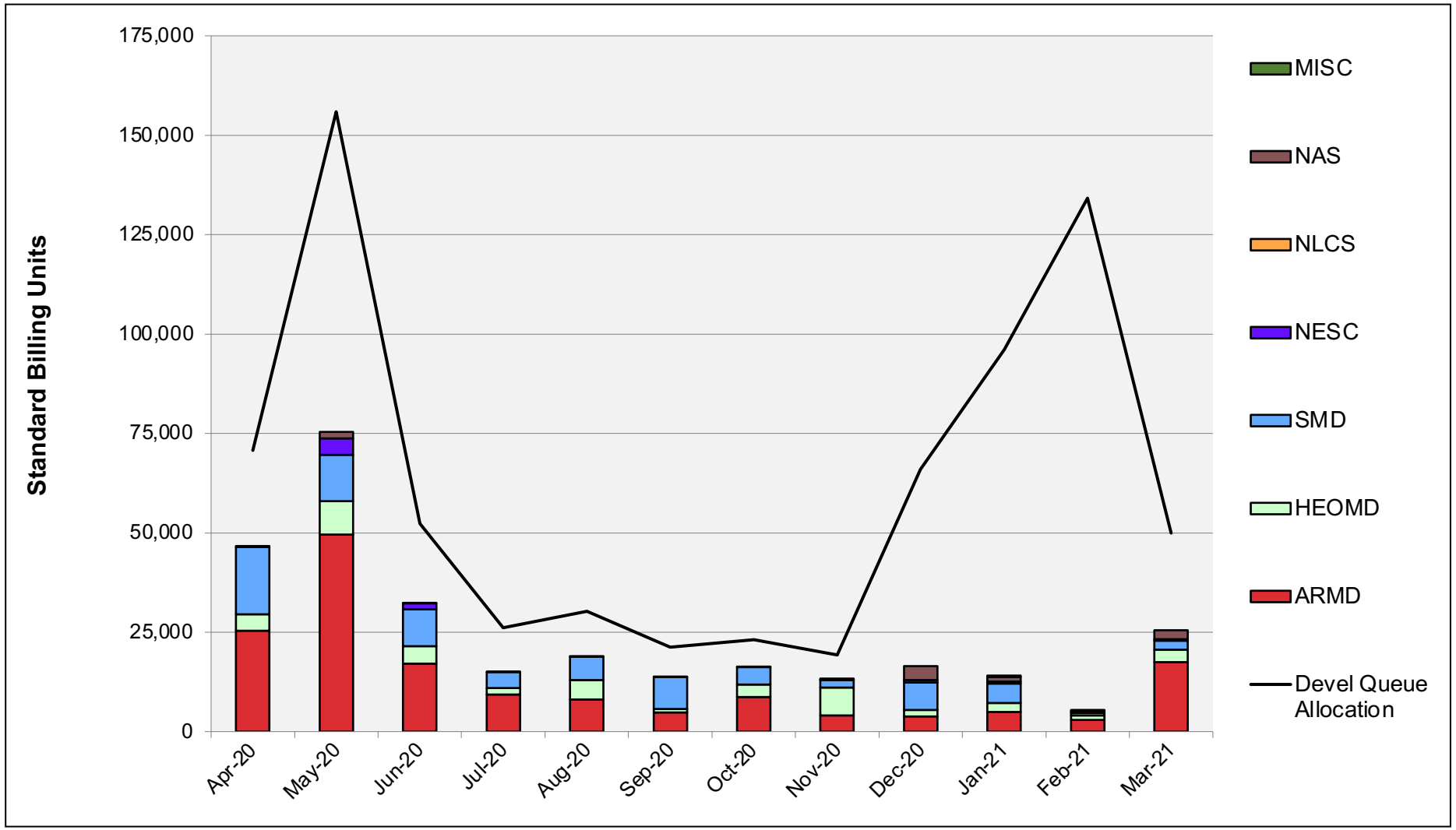

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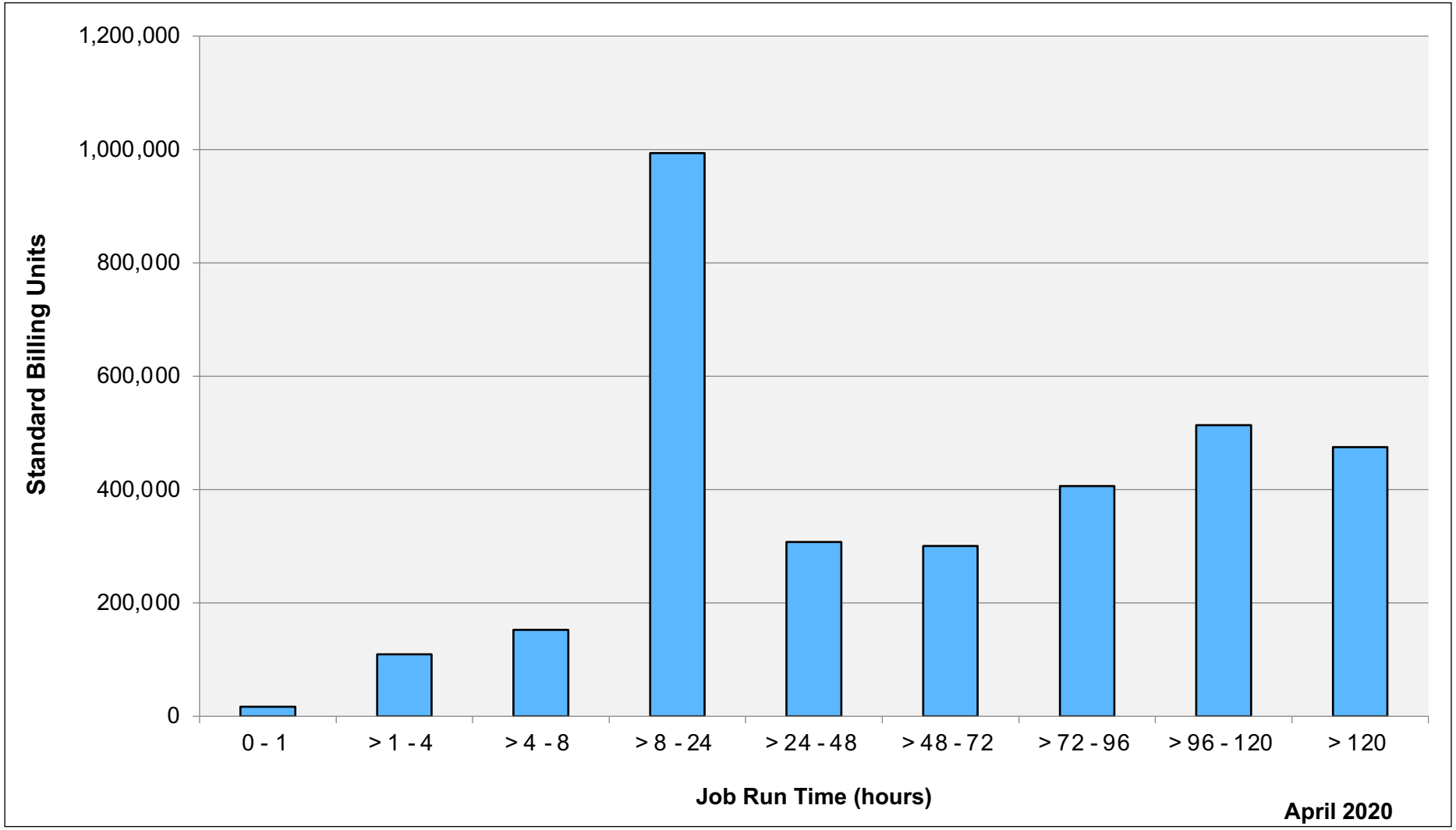
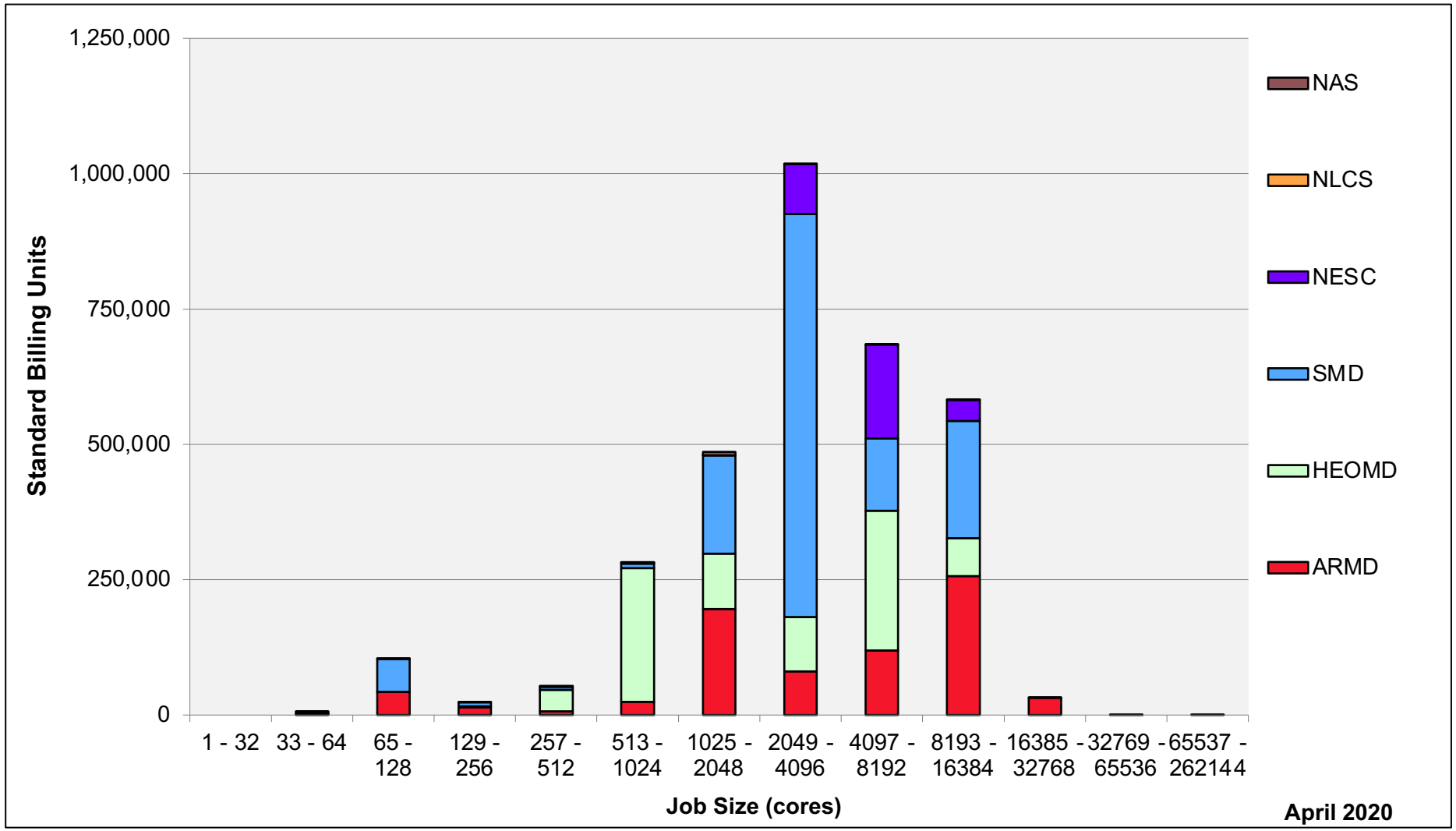
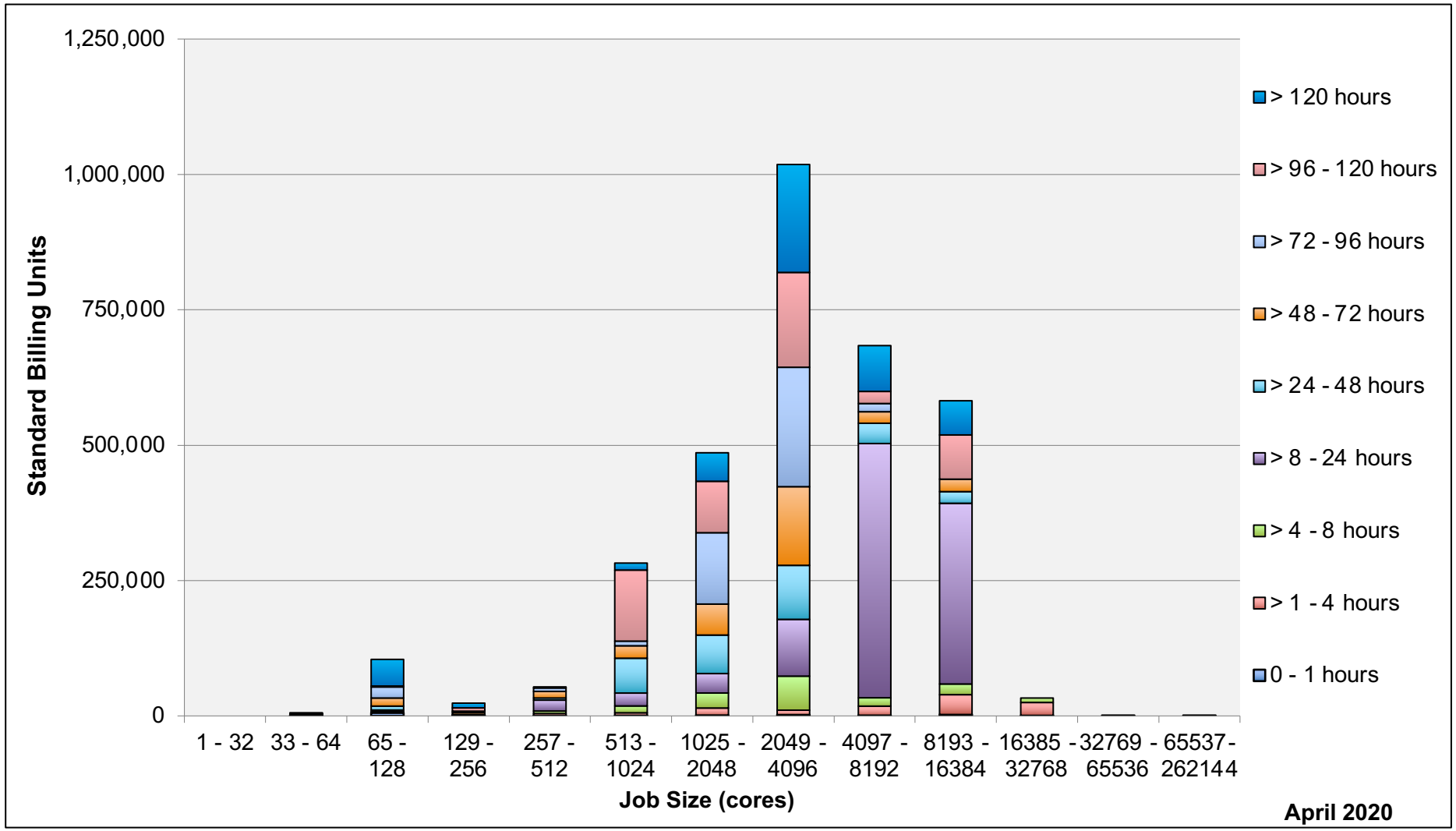


Aitken: Monthly Utilization by Job Size



Aitken: Monthly Utilization by Size and Length



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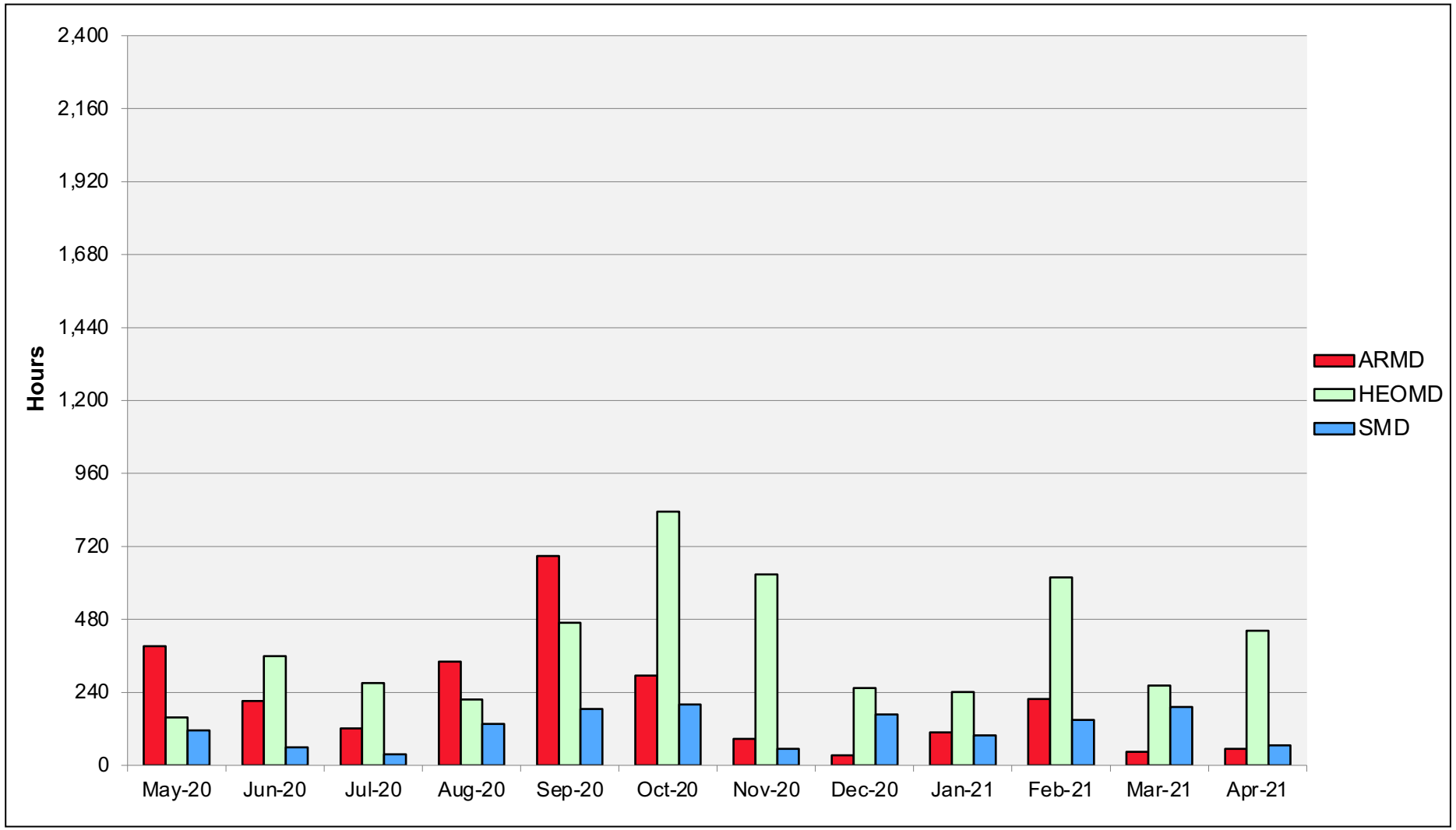
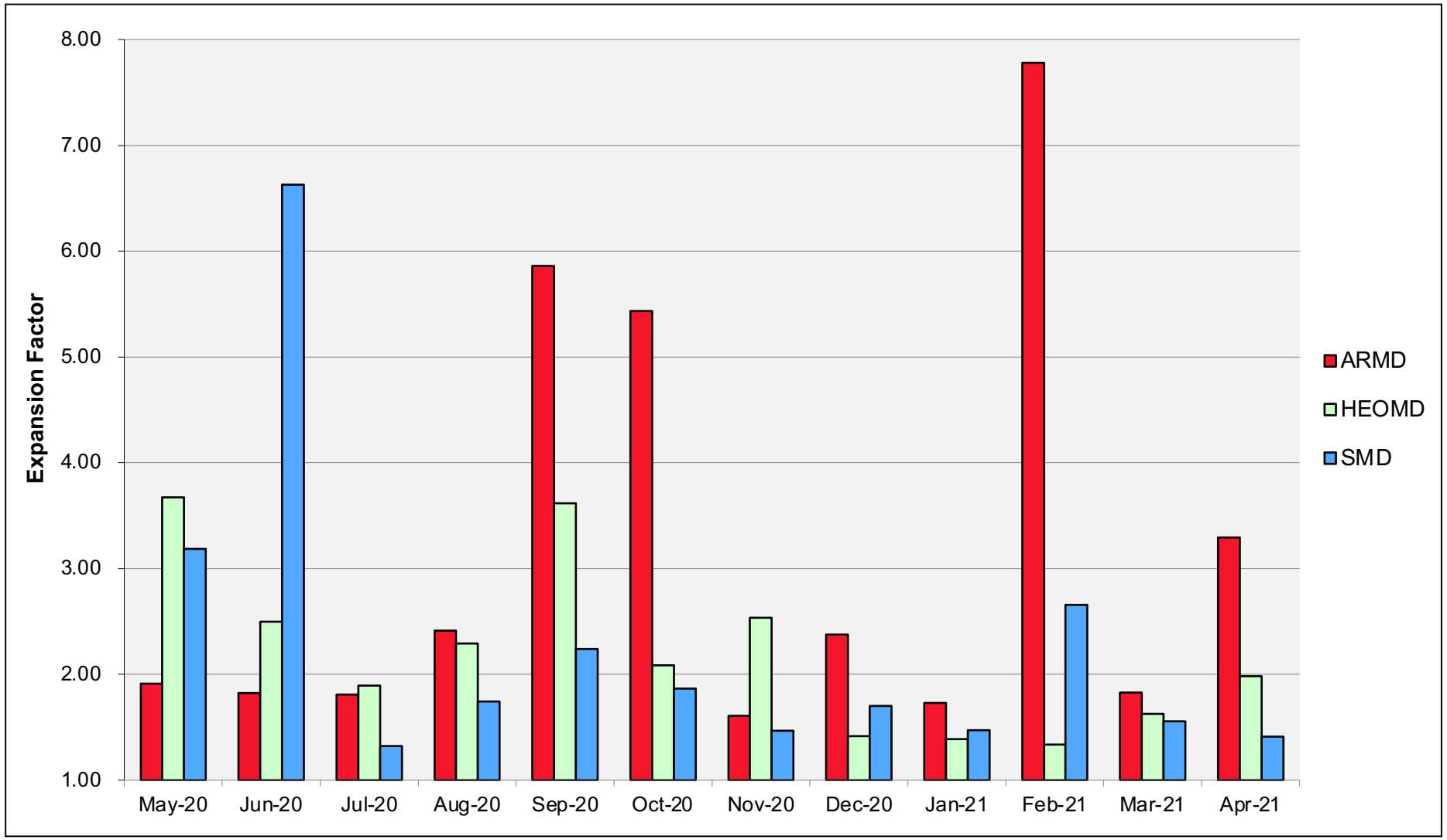
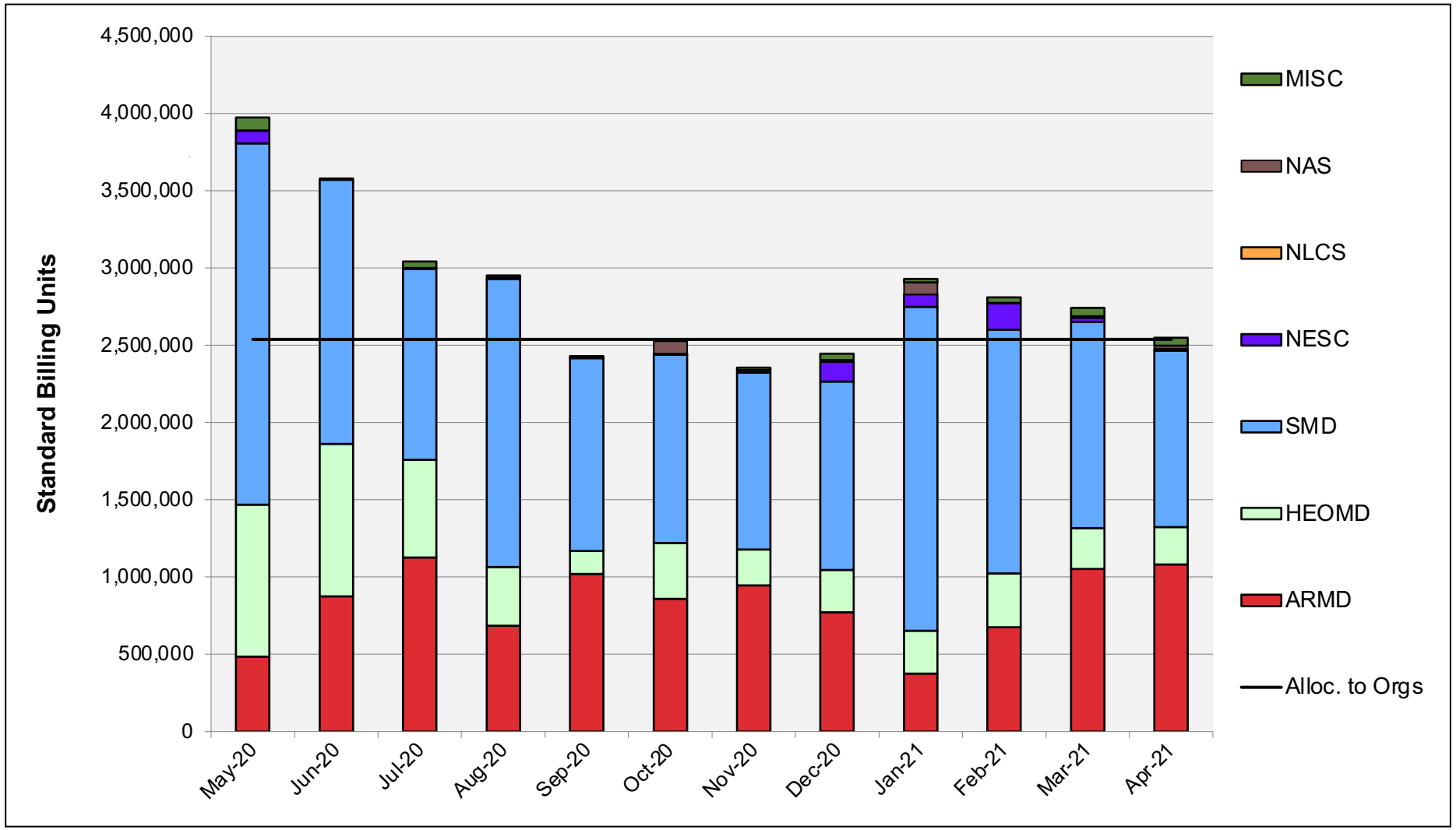


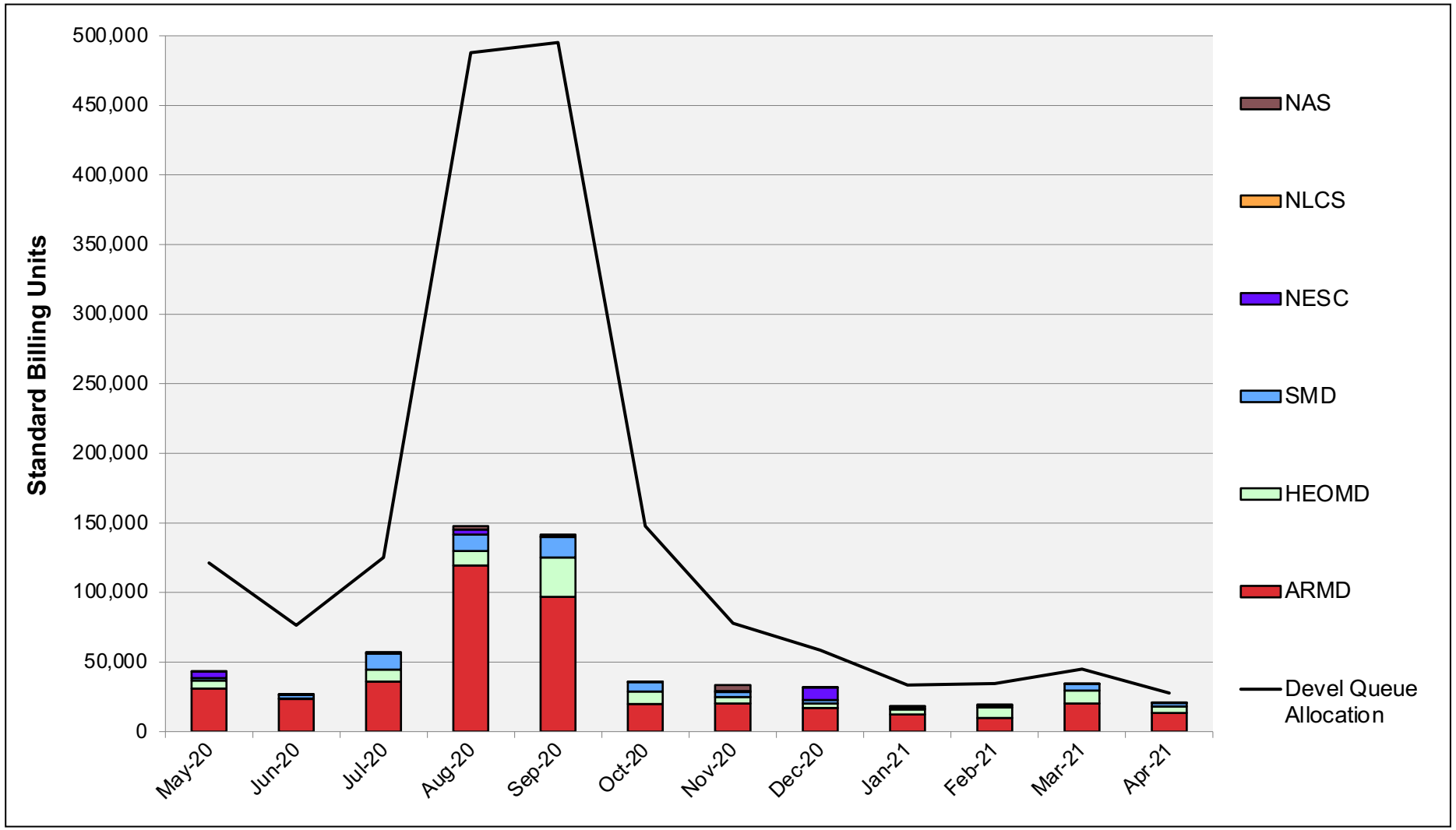
Aitken: Average Expansion Factor



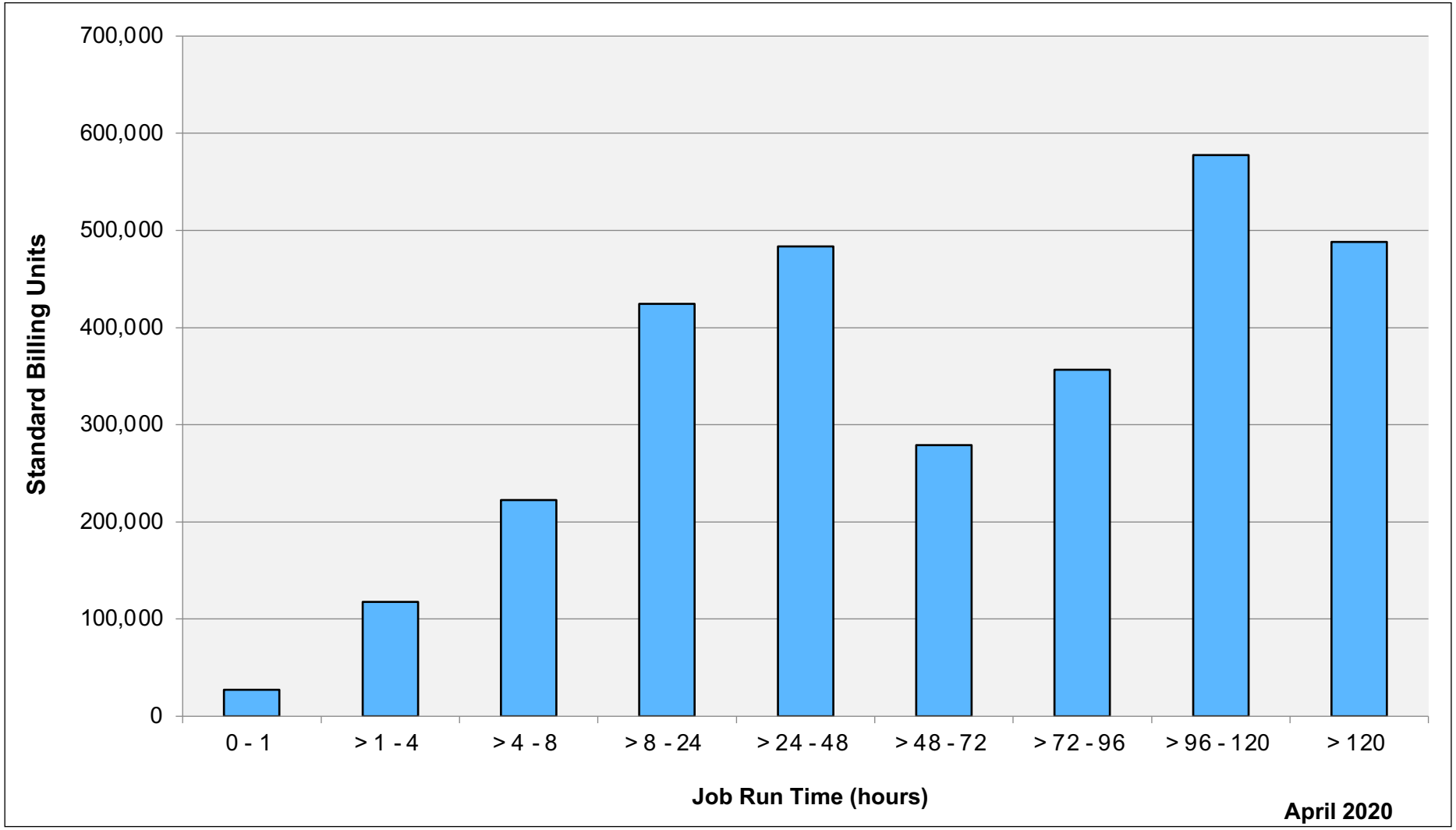
Electra: SBUs Reported, Normalized to 30-Day Month



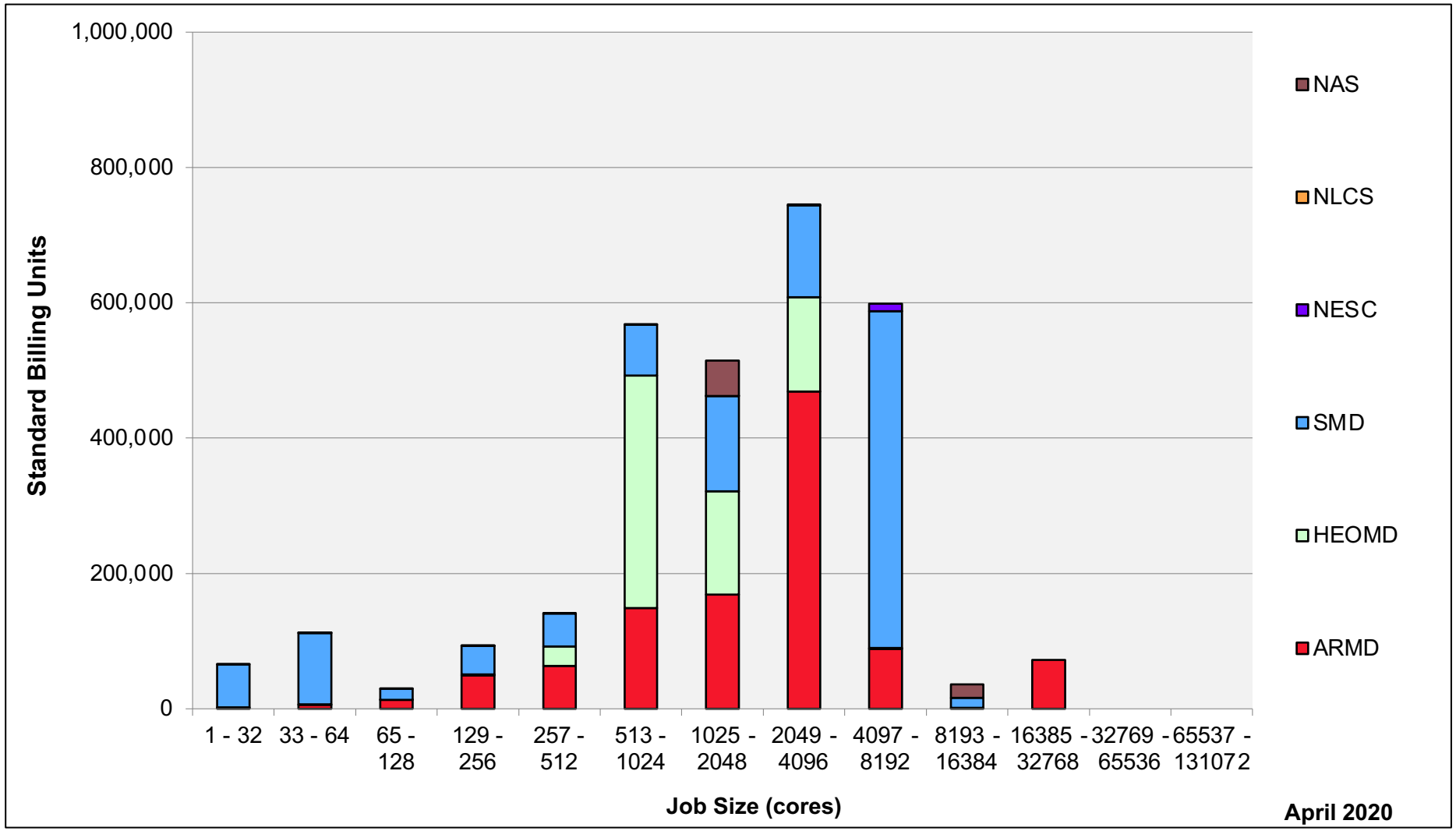
Electra: Devel Queue Utilization



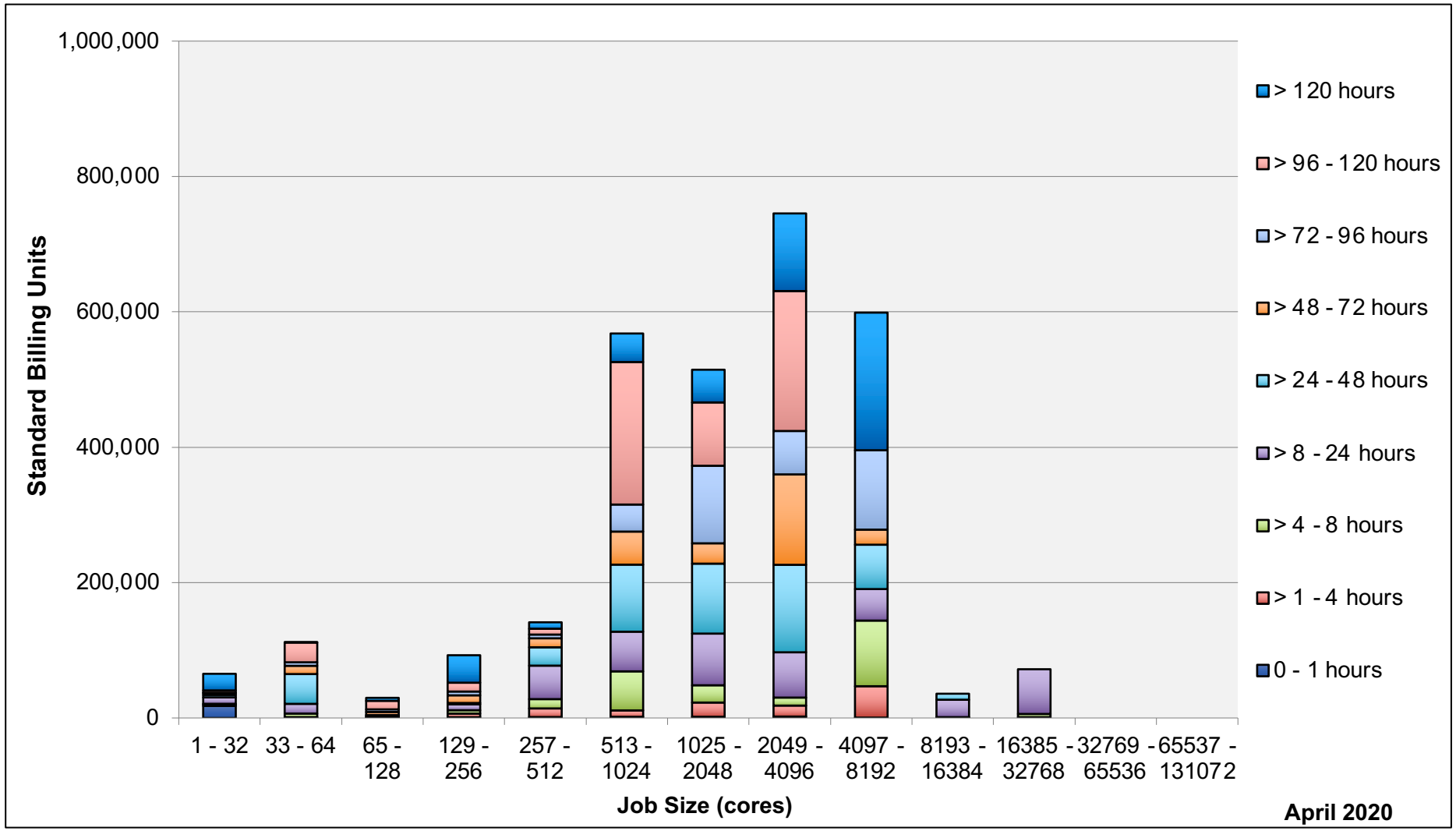
Electra: Monthly Utilization by Job Length



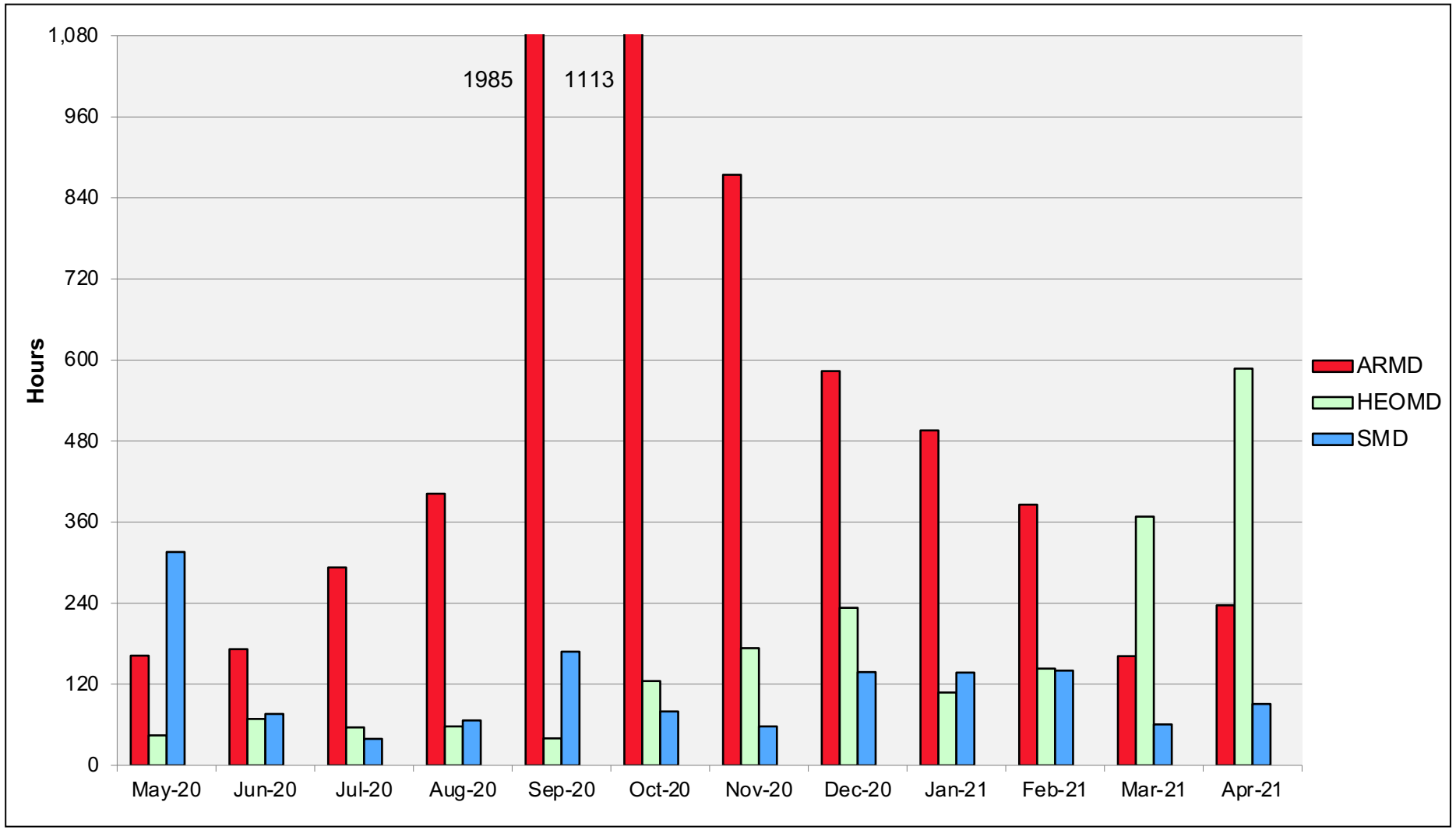
Electra: Monthly Utilization by Job Size



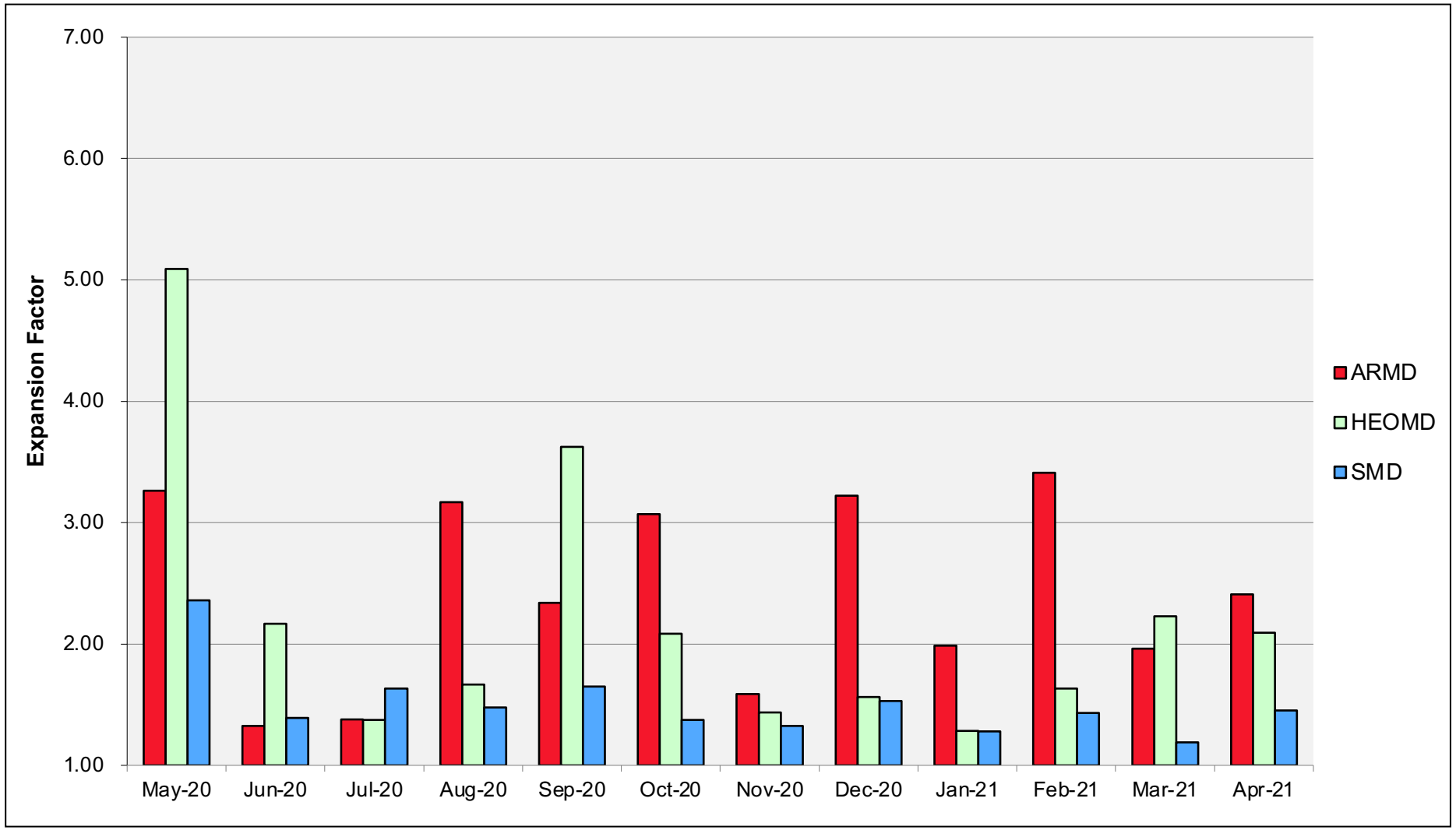
Electra: Monthly Utilization by Size and Length



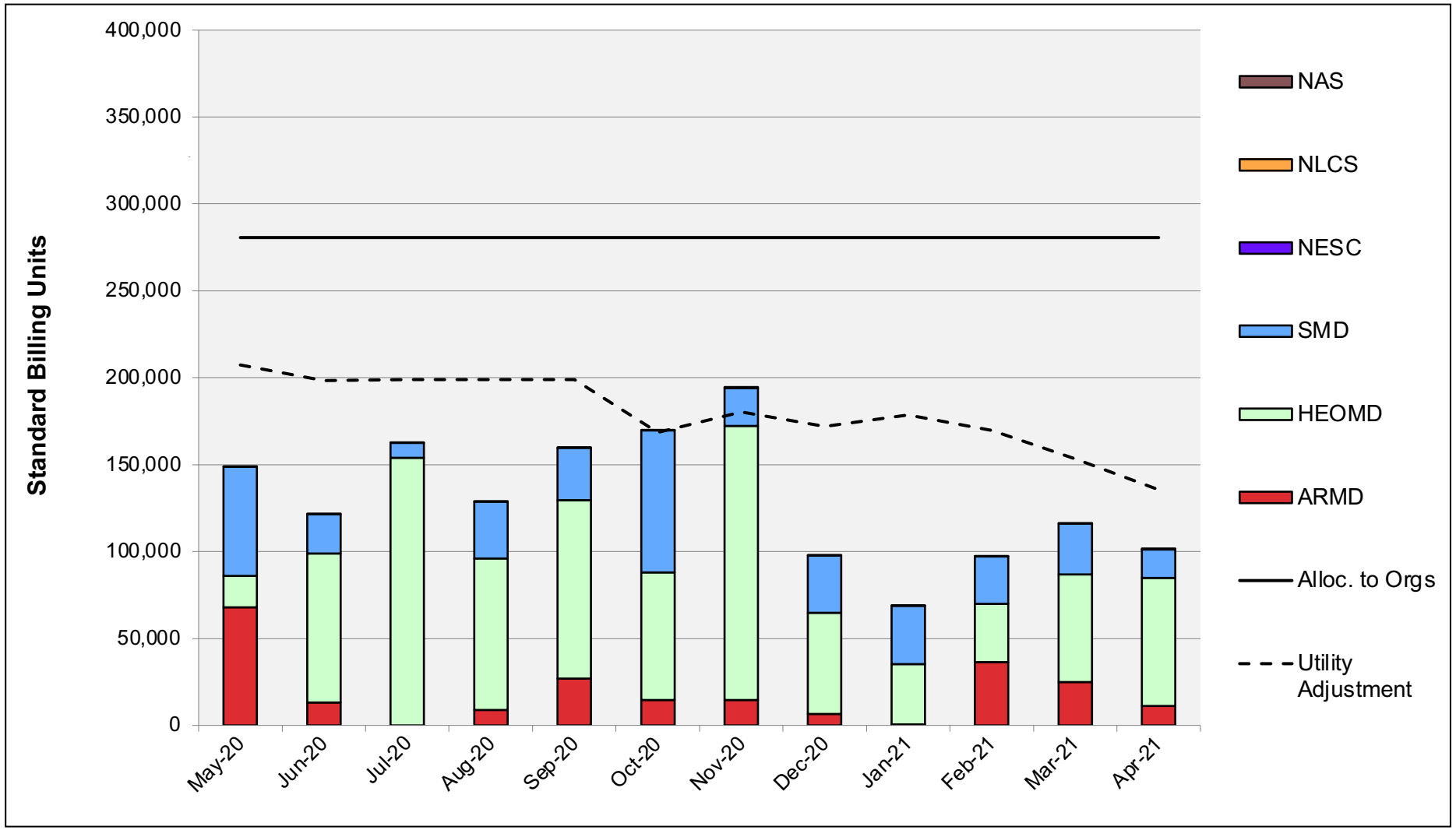
Electra: Average Time to Clear All Jobs



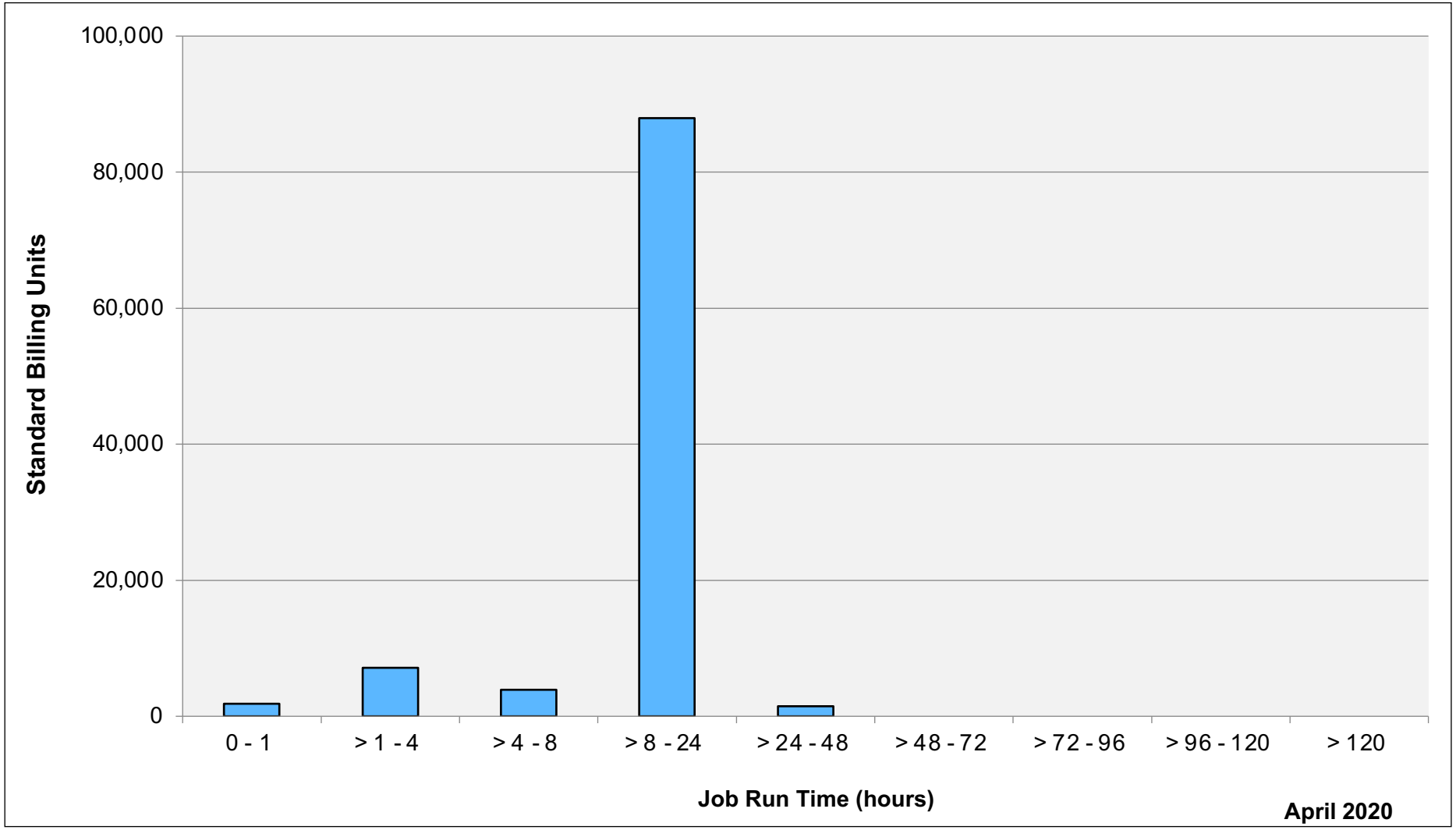
Electra: Average Expansion Factor



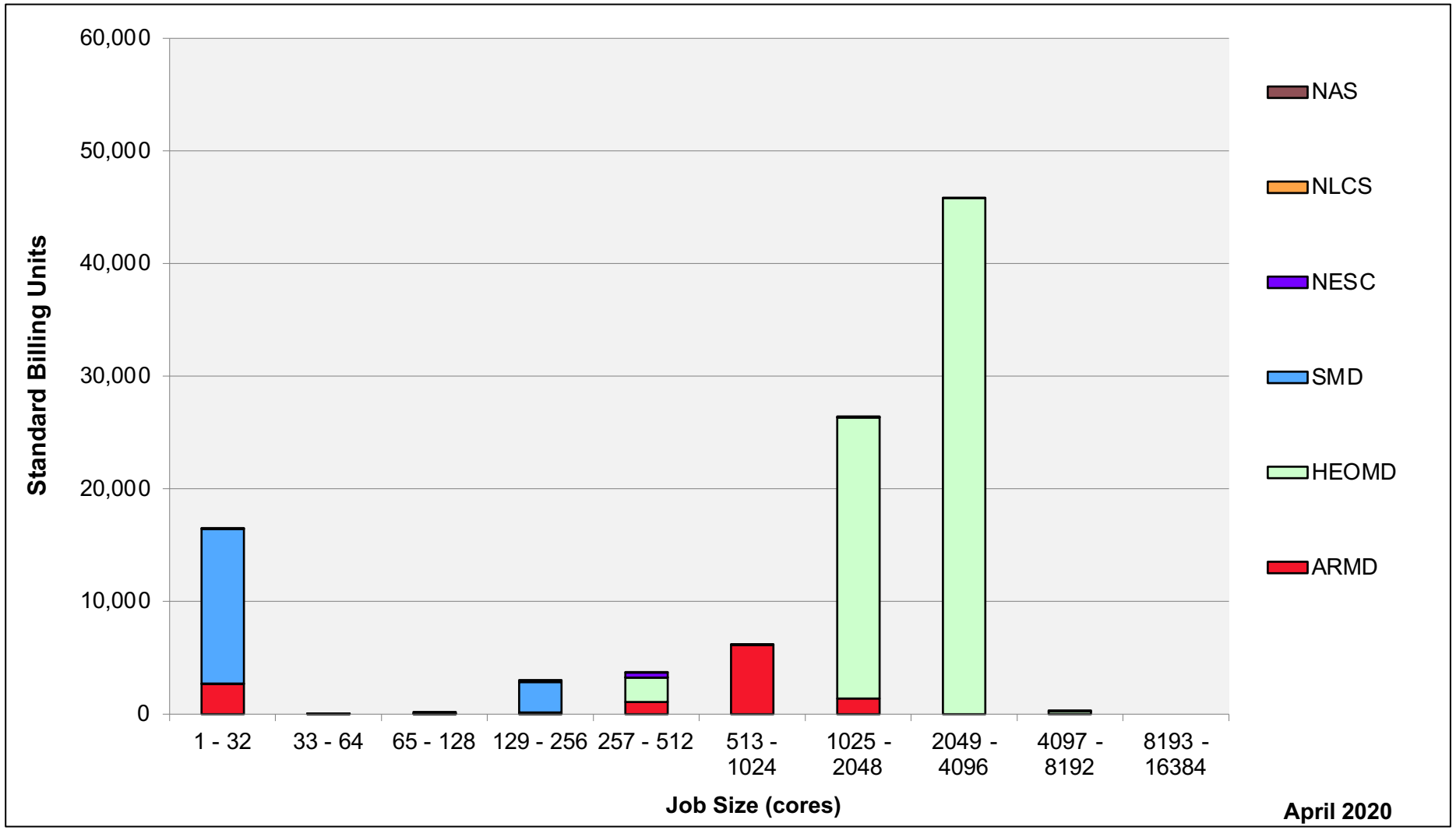
Merope: SBUs Reported, Normalized to 30-Day Month



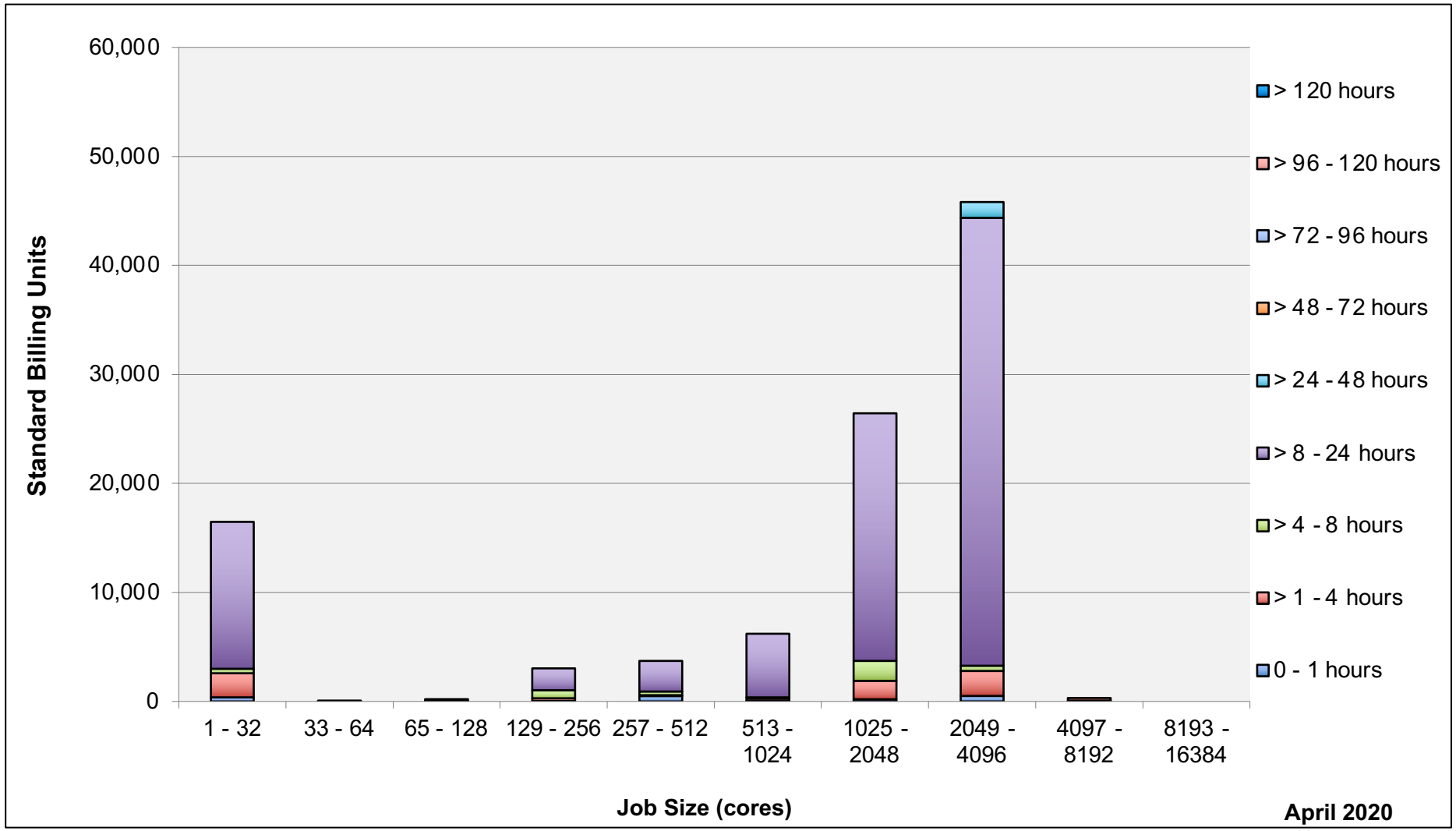
Merope: Monthly Utilization by Job Length



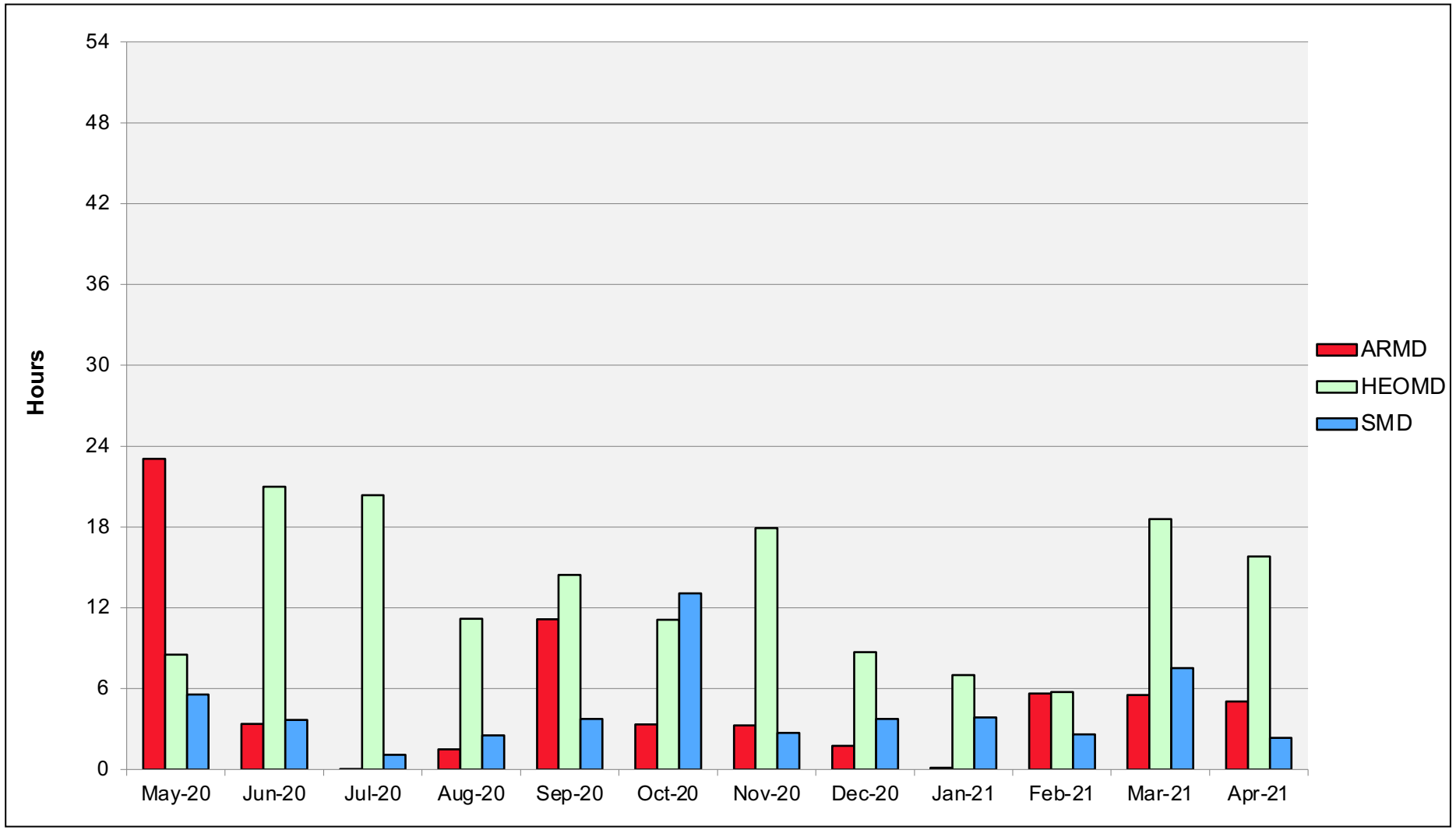
Merope: Monthly Utilization by Job Size



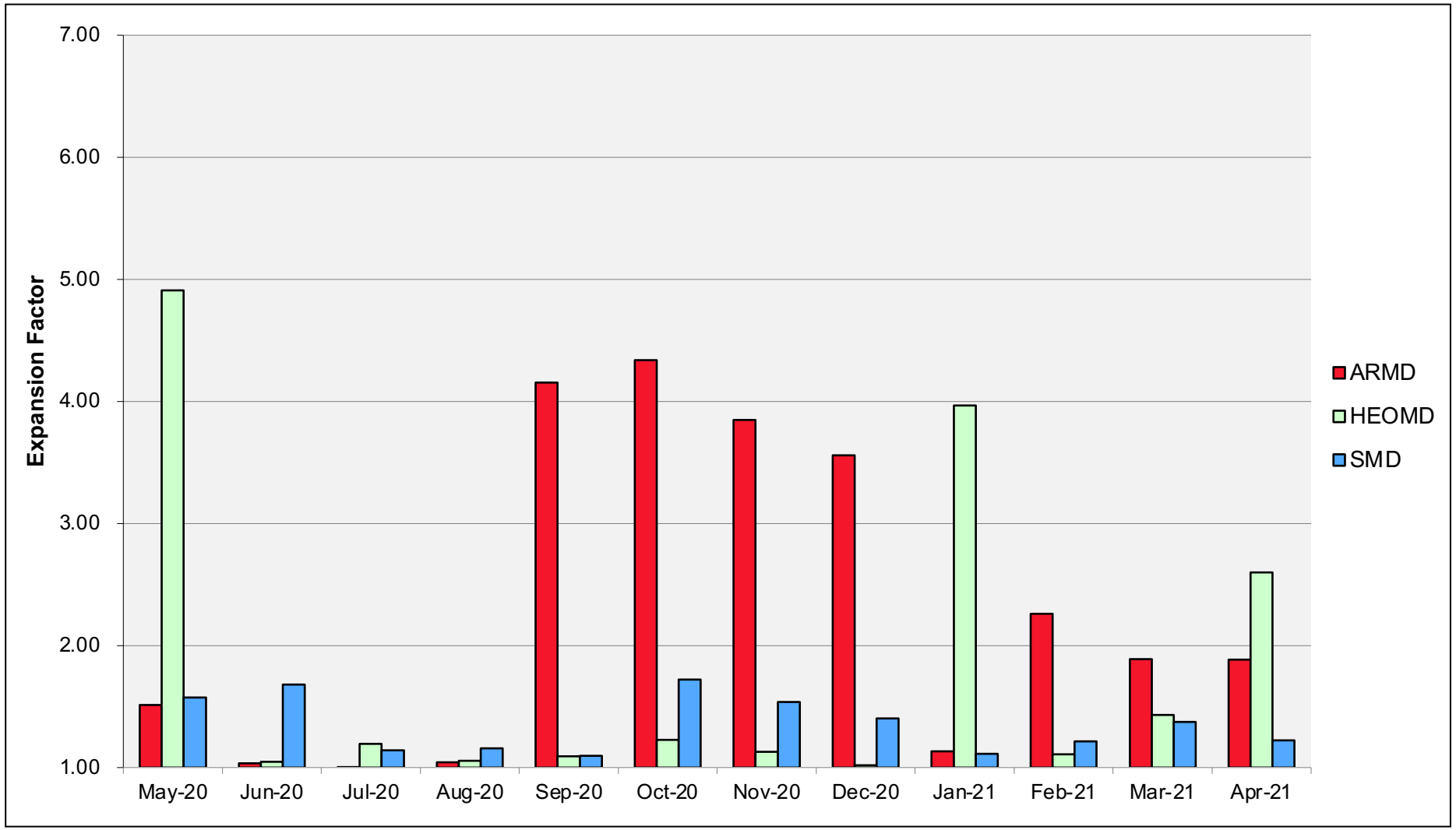
Merope: Monthly Utilization by Size and Length



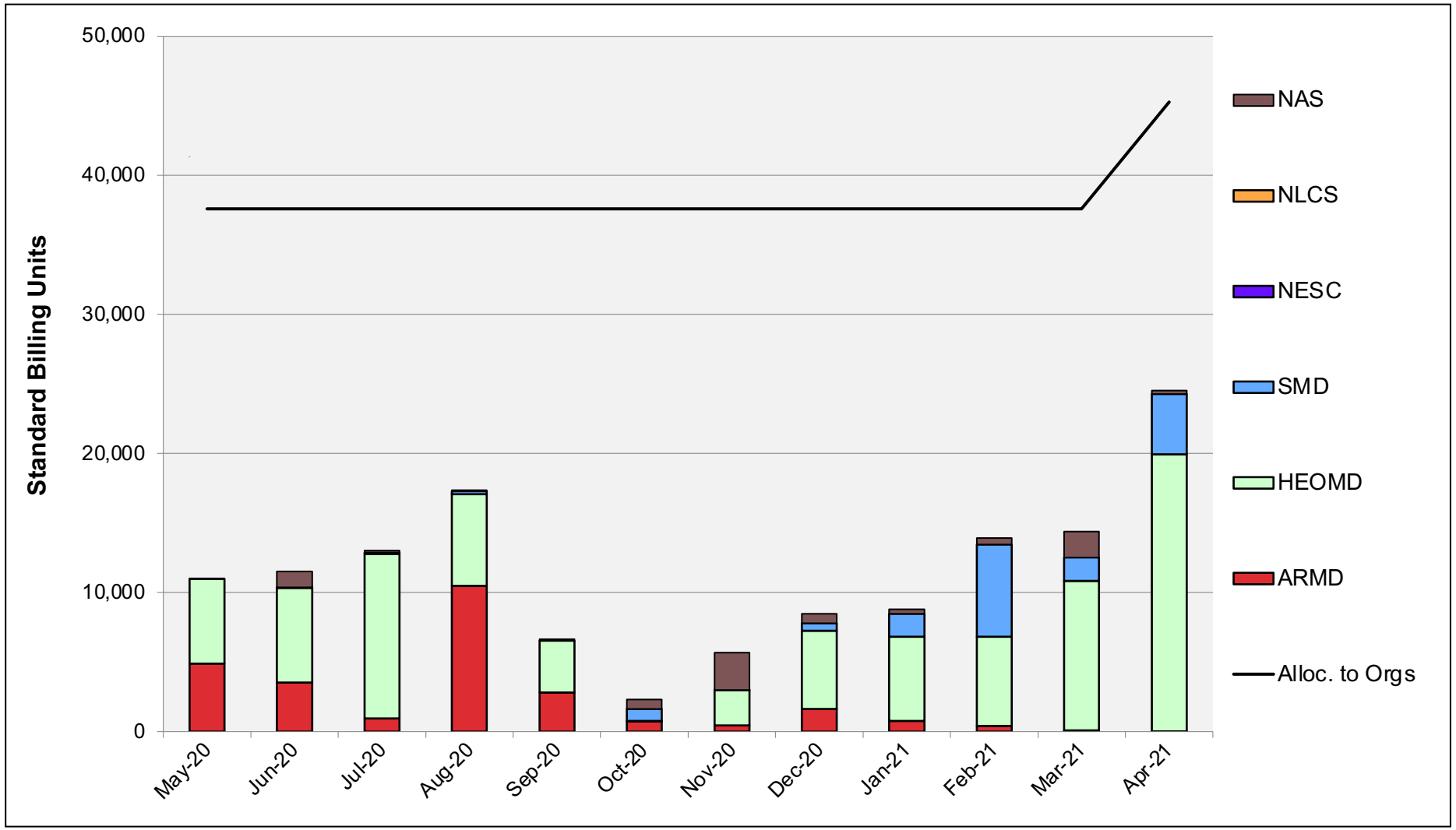
Merope: Average Time to Clear All Jobs



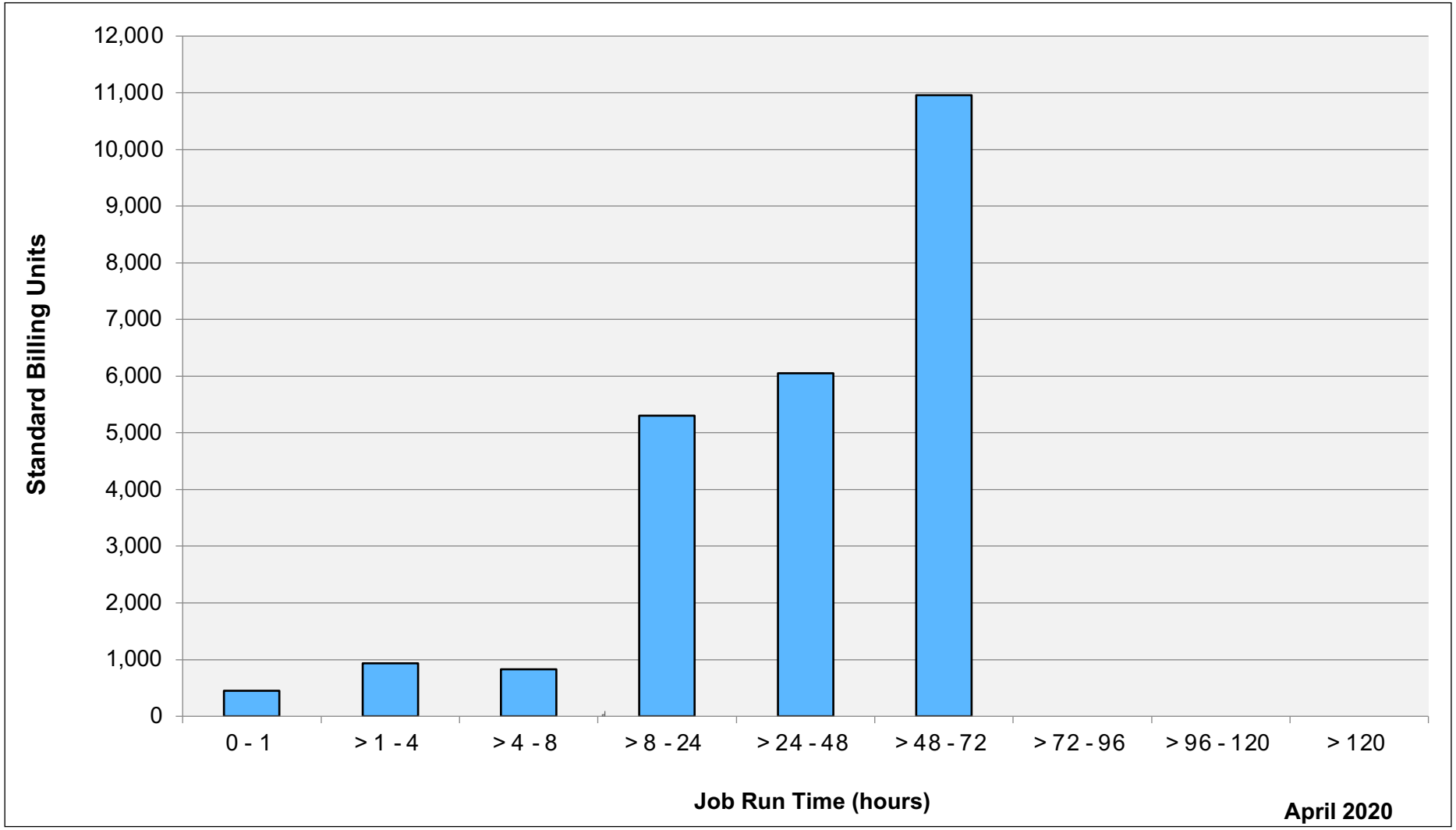
Merope: Average Expansion Factor



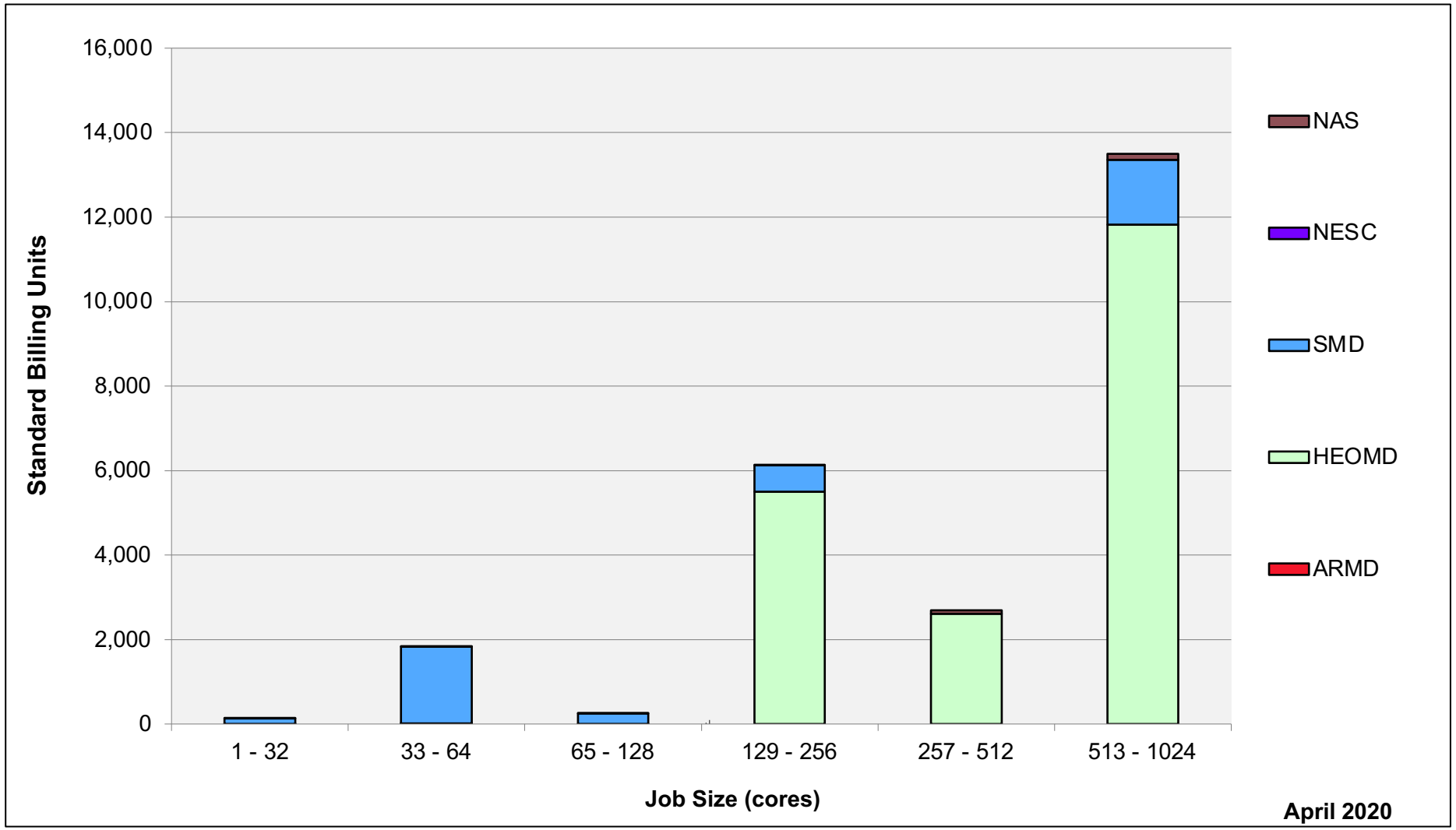
Endeavour: SBUs Reported, Normalized to 30-Day Month



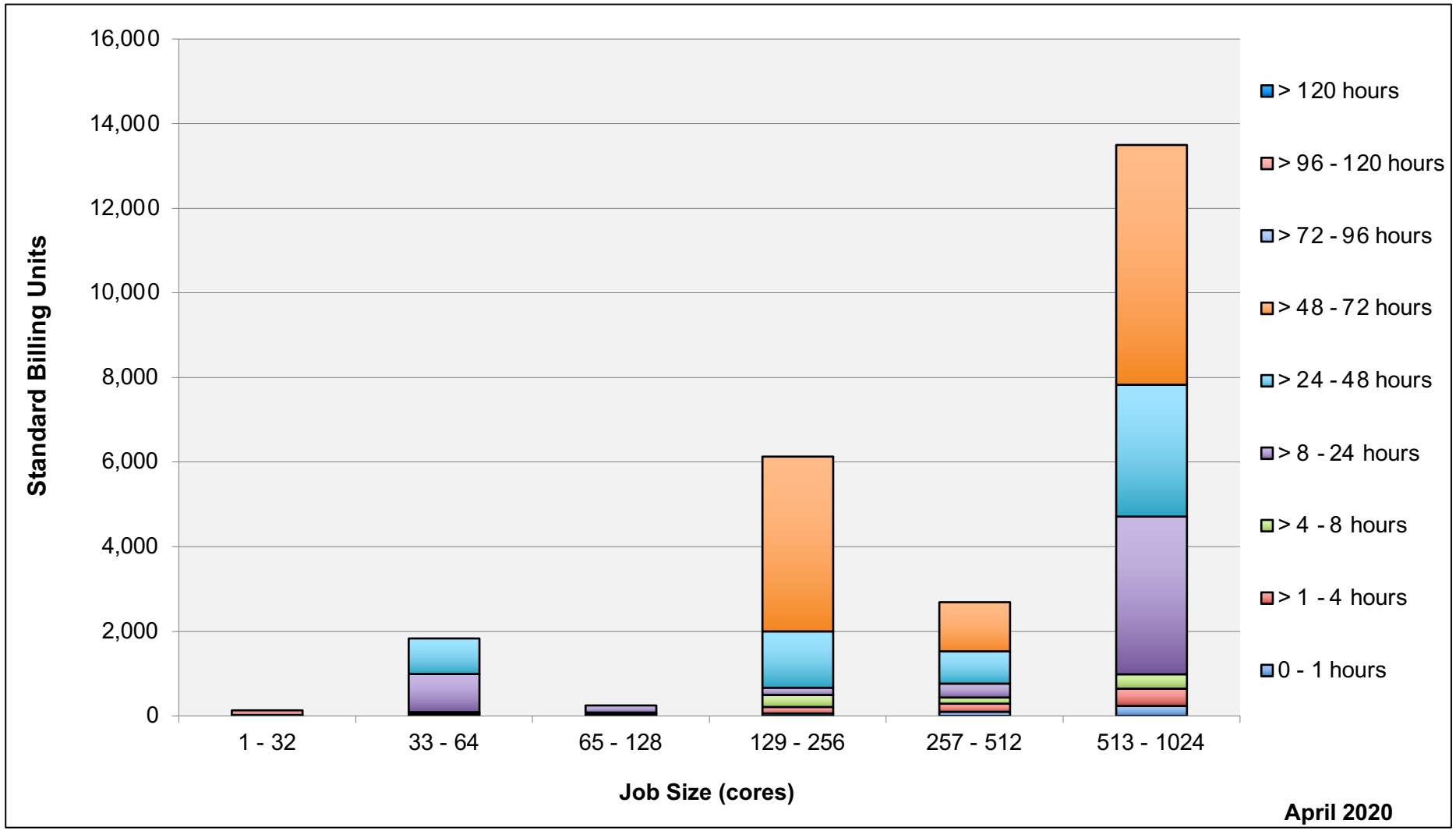
Endeavour: Monthly Utilization by Job Length



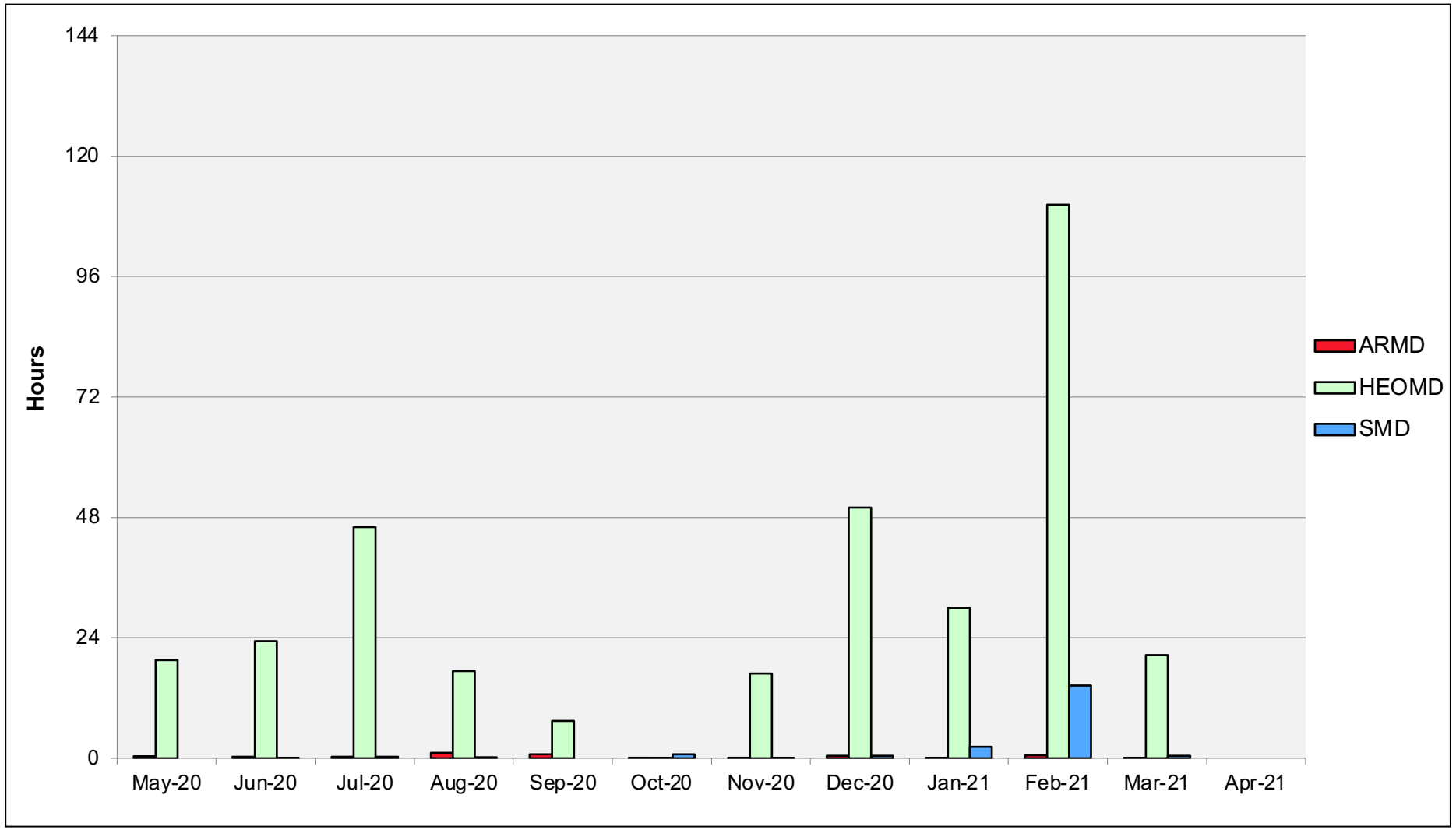
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor